



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:50 AM GMT

PDB ID : 3G1F  
Title : Crystal structure of orotidine 5'-monophosphate decarboxylase from Methanobacterium thermoautotrophicum complexed with 5,6-dihydroorotidine 5'-monophosphate  
Authors : Fedorov, A.A.; Fedorov, E.V.; Chan, K.K.; Gerlt, J.A.; Almo, S.C.  
Deposited on : 2009-01-29  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

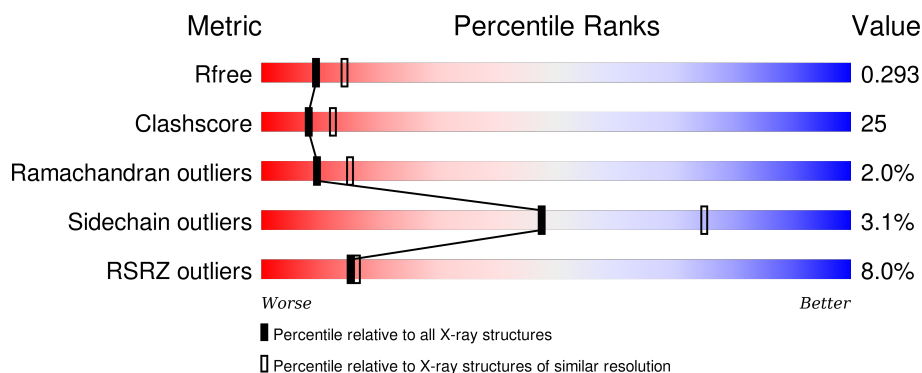
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	228	<div> <div>5%</div> <div>76% 18% . .</div> </div>
1	B	228	<div> <div>7%</div> <div>57% 34% . 5%</div> </div>
1	C	228	<div> <div>3%</div> <div>74% 20% . .</div> </div>
1	D	228	<div> <div>8%</div> <div>52% 39% . 6%</div> </div>
1	E	228	<div> <div>5%</div> <div>47% 46% . 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	228	
1	G	228	
1	H	228	
1	I	228	
1	J	228	
1	K	228	
1	L	228	
1	M	228	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21732 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1668	1048	291	317	12			
1	B	216	Total	C	N	O	S	0	0	0
			1638	1029	287	311	11			
1	C	218	Total	C	N	O	S	0	0	0
			1653	1039	289	313	12			
1	D	215	Total	C	N	O	S	0	0	0
			1630	1025	286	308	11			
1	E	217	Total	C	N	O	S	0	0	0
			1646	1034	288	312	12			
1	F	217	Total	C	N	O	S	0	0	0
			1646	1034	288	312	12			
1	G	217	Total	C	N	O	S	0	0	0
			1646	1034	288	312	12			
1	H	216	Total	C	N	O	S	0	0	0
			1638	1029	287	311	11			
1	I	212	Total	C	N	O	S	0	0	0
			1607	1011	282	304	10			
1	J	218	Total	C	N	O	S	0	0	0
			1653	1039	289	313	12			
1	K	216	Total	C	N	O	S	0	0	0
			1638	1029	287	311	11			
1	L	216	Total	C	N	O	S	0	0	0
			1638	1029	287	311	11			
1	M	217	Total	C	N	O	S	0	0	0
			1646	1034	288	312	12			

There are 13 discrepancies between the modelled and reference sequences:

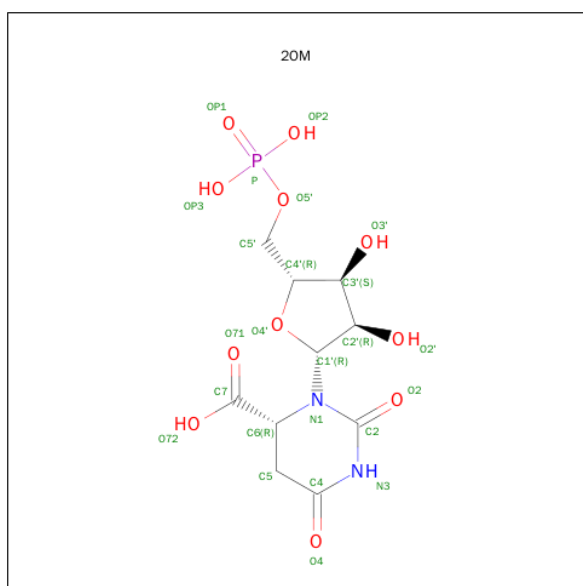
Chain	Residue	Modelled	Actual	Comment	Reference
A	101	PRO	ARG	ENGINEERED	UNP O26232
B	101	PRO	ARG	ENGINEERED	UNP O26232
C	101	PRO	ARG	ENGINEERED	UNP O26232

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Chain	Residue	Modelled	Actual	Comment	Reference
D	101	PRO	ARG	ENGINEERED	UNP O26232
E	101	PRO	ARG	ENGINEERED	UNP O26232
F	101	PRO	ARG	ENGINEERED	UNP O26232
G	101	PRO	ARG	ENGINEERED	UNP O26232
H	101	PRO	ARG	ENGINEERED	UNP O26232
I	101	PRO	ARG	ENGINEERED	UNP O26232
J	101	PRO	ARG	ENGINEERED	UNP O26232
K	101	PRO	ARG	ENGINEERED	UNP O26232
L	101	PRO	ARG	ENGINEERED	UNP O26232
M	101	PRO	ARG	ENGINEERED	UNP O26232

- Molecule 2 is 5,6-DIHYDROOROTIDINE 5'-MONOPHOSPHATE (three-letter code: 2OM) (formula:  $C_{10}H_{15}N_2O_{11}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	B	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	C	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	D	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	E	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	F	1	Total	C	N	O	P	0	0
			24	10	2	11	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	H	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	I	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	J	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	K	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	L	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	M	1	Total	C	N	O	P	0	0
			24	10	2	11	1		

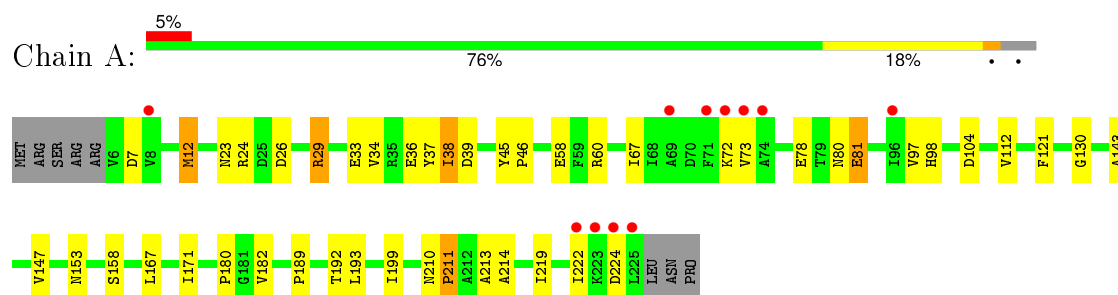
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	9	Total	O	0	0
			9	9		
3	C	9	Total	O	0	0
			9	9		
3	D	11	Total	O	0	0
			11	11		
3	E	2	Total	O	0	0
			2	2		
3	F	1	Total	O	0	0
			1	1		
3	G	2	Total	O	0	0
			2	2		
3	I	7	Total	O	0	0
			7	7		
3	J	6	Total	O	0	0
			6	6		
3	M	9	Total	O	0	0
			9	9		

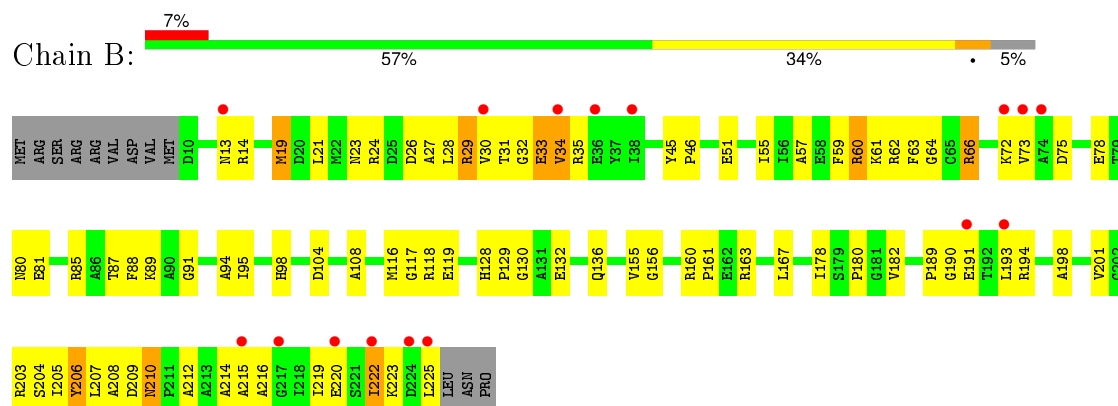
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

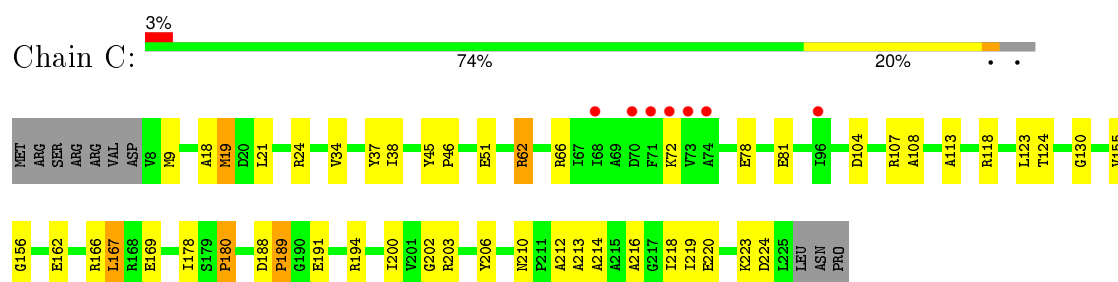
#### • Molecule 1: Orotidine 5'-phosphate decarboxylase



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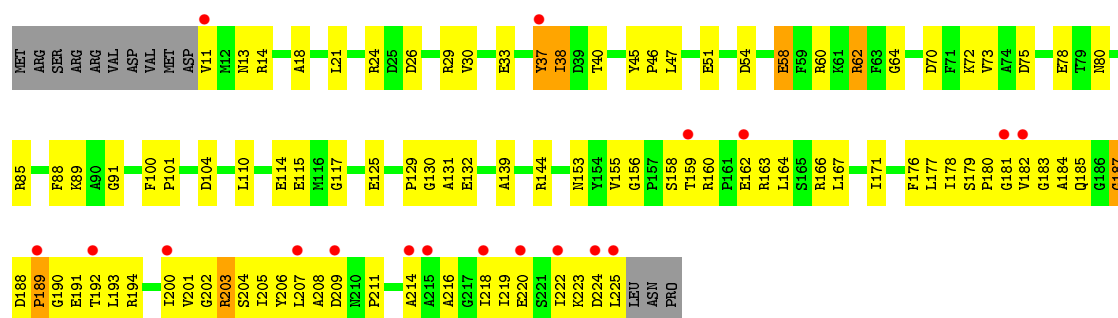


#### • Molecule 1: Orotidine 5'-phosphate decarboxylase

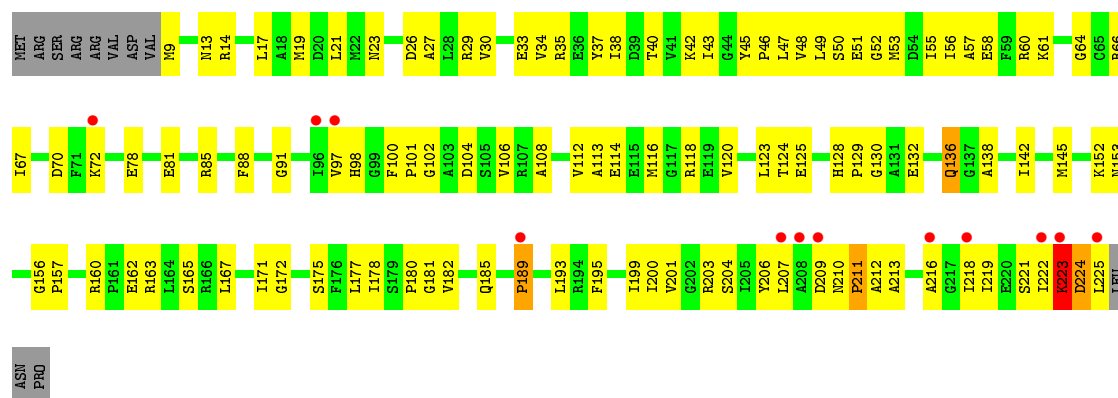


#### • Molecule 1: Orotidine 5'-phosphate decarboxylase

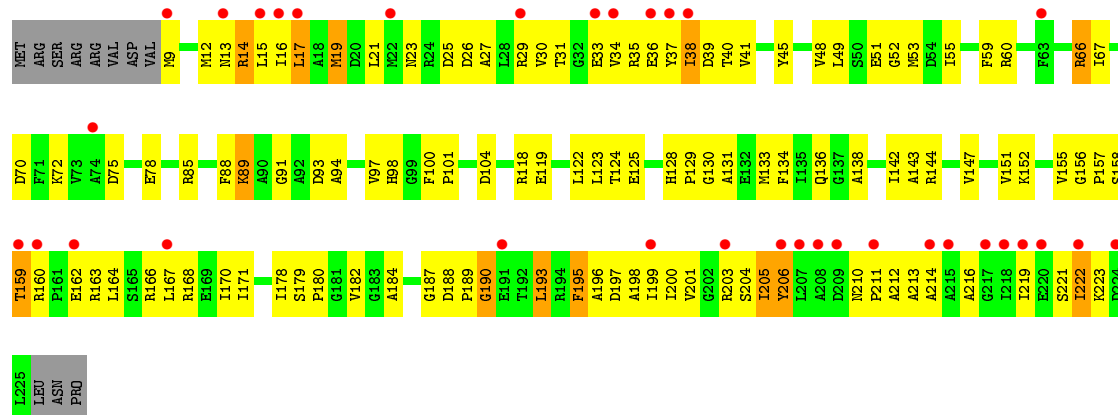




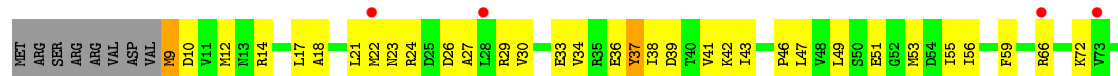
- Molecule 1: Orotidine 5'-phosphate decarboxylase



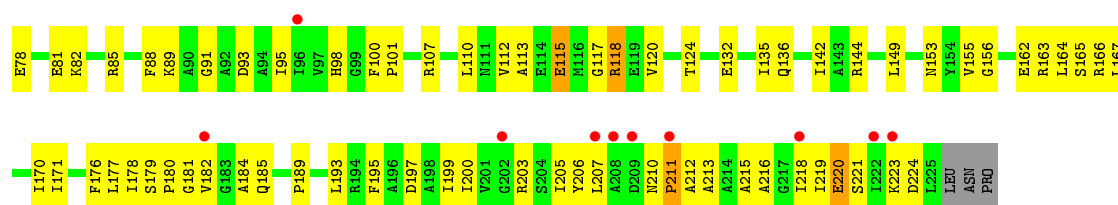
- Molecule 1: Orotidine 5'-phosphate decarboxylase



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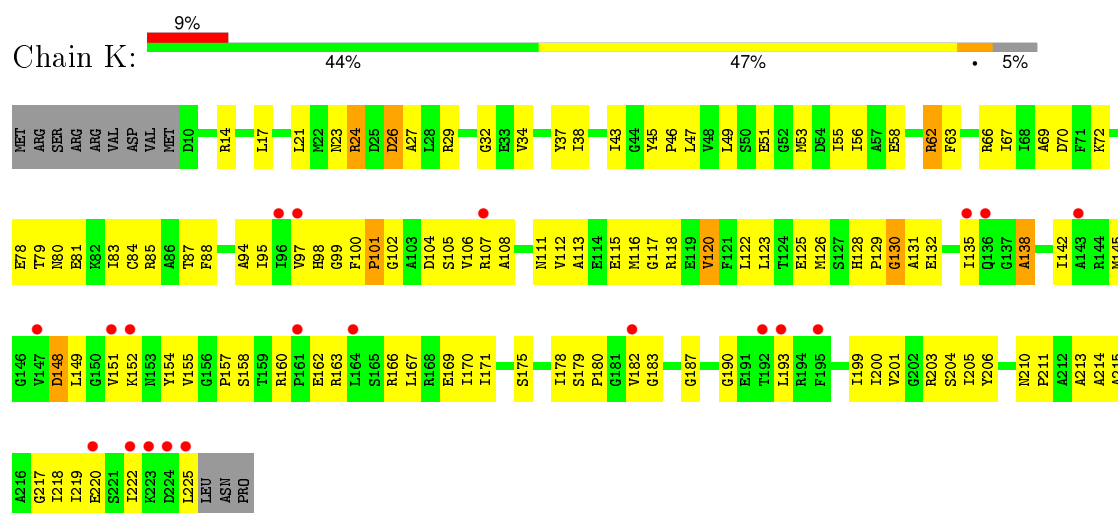
• Molecule 1: Orotidine 5'-phosphate decarboxylase



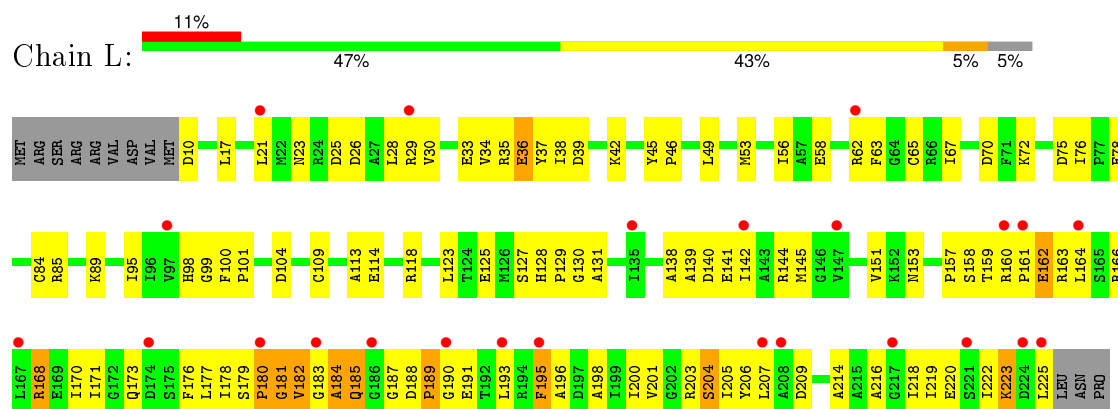
• Molecule 1: Orotidine 5'-phosphate decarboxylase



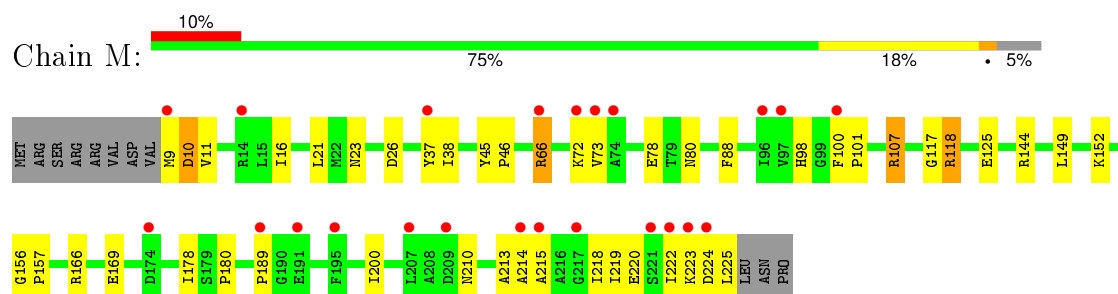
• Molecule 1: Orotidine 5'-phosphate decarboxylase



- Molecule 1: Orotidine 5'-phosphate decarboxylase



- Molecule 1: Orotidine 5'-phosphate decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.61Å 101.71Å 192.08Å 90.00° 91.49° 90.00°	Depositor
Resolution (Å)	24.98 – 2.50 38.17 – 2.08	Depositor EDS
% Data completeness (in resolution range)	96.4 (24.98-2.50) 90.8 (38.17-2.08)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.243 , 0.294 0.242 , 0.293	Depositor DCC
$R_{free}$ test set	4766 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.0	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 153661 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2OM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.50	0/1691	0.71	0/2282
1	B	0.49	0/1661	0.68	0/2241
1	C	0.44	0/1676	0.65	0/2261
1	D	0.43	0/1653	0.66	0/2230
1	E	0.36	0/1669	0.59	0/2251
1	F	0.38	0/1669	0.63	0/2251
1	G	0.37	0/1669	0.59	0/2251
1	H	0.35	0/1661	0.58	0/2241
1	I	0.40	0/1630	0.62	0/2199
1	J	0.40	0/1676	0.61	0/2261
1	K	0.33	0/1661	0.56	0/2241
1	L	0.33	0/1661	0.57	0/2241
1	M	0.53	0/1669	1.28	6/2251 (0.3%)
All	All	0.41	0/21646	0.70	6/29201 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	144	ARG	NE-CZ-NH1	-29.46	105.57	120.30
1	M	66	ARG	CA-CB-CG	26.24	171.12	113.40
1	M	144	ARG	NE-CZ-NH2	25.00	132.80	120.30
1	M	118	ARG	CG-CD-NE	18.54	150.73	111.80
1	M	144	ARG	CD-NE-CZ	13.54	142.55	123.60
1	M	144	ARG	CG-CD-NE	-7.41	96.23	111.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1668	0	1682	38	0
1	B	1638	0	1651	89	0
1	C	1653	0	1669	44	0
1	D	1630	0	1647	94	0
1	E	1646	0	1660	115	0
1	F	1646	0	1660	137	0
1	G	1646	0	1660	102	0
1	H	1638	0	1651	77	0
1	I	1607	0	1623	91	0
1	J	1653	0	1669	80	0
1	K	1638	0	1651	122	0
1	L	1638	0	1651	115	0
1	M	1646	0	1660	39	0
2	A	24	0	12	2	0
2	B	24	0	12	3	0
2	C	24	0	12	1	0
2	D	24	0	12	2	0
2	E	24	0	12	2	0
2	F	24	0	12	3	0
2	G	24	0	12	2	0
2	H	24	0	12	1	0
2	I	24	0	12	0	0
2	J	24	0	12	2	0
2	K	24	0	12	2	0
2	L	24	0	12	2	0
2	M	24	0	12	2	0
3	A	17	0	0	0	0
3	B	9	0	0	0	0
3	C	9	0	0	0	0
3	D	11	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	I	7	0	0	1	0
3	J	6	0	0	0	0
3	M	9	0	0	0	0
All	All	21732	0	21690	1069	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1069) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ARG:HH11	1:C:62:ARG:HB3	1.13	1.10
1:K:193:LEU:HD12	1:K:222:ILE:HG12	1.37	1.05
1:C:210:ASN:HD22	1:C:213:ALA:HB2	1.24	1.02
1:J:163:ARG:HH11	1:J:163:ARG:HA	1.25	1.02
1:L:168:ARG:HG3	1:L:173:GLN:HE22	1.24	1.01
1:F:66:ARG:HH11	1:F:66:ARG:HB3	1.22	1.01
1:E:189:PRO:HB2	1:E:222:ILE:HD11	1.38	1.01
1:A:29:ARG:HH11	1:A:29:ARG:HG3	1.28	0.99
1:B:136:GLN:HE21	1:B:163:ARG:HE	1.06	0.95
1:J:210:ASN:HD22	1:J:213:ALA:HB2	1.32	0.94
1:D:156:GLY:O	1:D:180:PRO:HD2	1.67	0.92
1:F:182:VAL:HA	1:F:187:GLY:HA3	1.49	0.91
1:E:61:LYS:HD2	1:G:9:MET:HA	1.51	0.91
1:F:193:LEU:HD21	1:F:222:ILE:HG12	1.52	0.89
1:C:62:ARG:HB3	1:C:62:ARG:NH1	1.88	0.88
1:C:210:ASN:ND2	1:C:213:ALA:HB2	1.89	0.88
1:E:78:GLU:HG2	1:F:203:ARG:NH1	1.88	0.88
1:E:128:HIS:HB2	1:E:129:PRO:HD2	1.54	0.87
1:H:210:ASN:HD22	1:H:213:ALA:HB2	1.39	0.87
1:J:66:ARG:HH11	1:J:66:ARG:HB3	1.40	0.87
1:E:14:ARG:HE	1:E:193:LEU:HD13	1.41	0.85
1:F:160:ARG:HD3	1:F:163:ARG:HG3	1.59	0.84
1:E:171:ILE:HD13	1:E:175:SER:HB2	1.57	0.84
1:J:220:GLU:HA	1:J:223:LYS:HG2	1.58	0.84
1:L:158:SER:HB2	1:L:179:SER:HB3	1.57	0.84
1:B:193:LEU:HD12	1:B:222:ILE:HG12	1.58	0.83
1:F:219:ILE:HD11	1:F:223:LYS:NZ	1.94	0.83
1:F:66:ARG:NH1	1:F:66:ARG:HB3	1.93	0.83
1:H:156:GLY:O	1:H:180:PRO:HD2	1.78	0.83
1:B:23:ASN:HB3	1:B:26:ASP:HB2	1.59	0.83
1:K:26:ASP:HA	1:K:29:ARG:HH12	1.44	0.82
1:C:62:ARG:CB	1:C:62:ARG:HH11	1.90	0.82
1:K:222:ILE:HD11	1:K:225:LEU:HD22	1.59	0.82
1:B:136:GLN:NE2	1:B:163:ARG:HE	1.78	0.82
1:J:72:LYS:HZ1	2:J:229:2OM:H6	1.44	0.82
1:I:160:ARG:HE	1:I:163:ARG:HG3	1.45	0.81
1:K:62:ARG:HH11	1:K:62:ARG:HB3	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:158:SER:HA	1:I:164:LEU:HD11	1.62	0.81
1:H:163:ARG:HA	1:H:163:ARG:HH11	1.44	0.81
1:F:156:GLY:O	1:F:180:PRO:HD2	1.81	0.81
1:G:30:VAL:HG13	1:G:211:PRO:HB3	1.61	0.80
1:F:193:LEU:HD11	1:F:222:ILE:HG21	1.62	0.80
1:H:164:LEU:HD23	1:H:195:PHE:HD1	1.46	0.80
1:D:38:ILE:HD12	1:D:40:THR:H	1.45	0.79
1:K:113:ALA:HB1	1:K:118:ARG:O	1.83	0.79
1:K:129:PRO:HG2	1:L:104:ASP:OD2	1.83	0.79
1:E:56:ILE:HG23	1:E:67:ILE:HG21	1.65	0.78
1:H:19:MET:HG3	1:H:47:LEU:HD22	1.66	0.78
1:L:168:ARG:HG3	1:L:173:GLN:NE2	1.97	0.77
1:H:138:ALA:O	1:H:142:ILE:HG13	1.84	0.77
1:M:9:MET:O	1:M:9:MET:HG3	1.85	0.77
1:M:189:PRO:HB3	1:M:222:ILE:HD11	1.66	0.77
1:E:37:TYR:HB3	1:E:219:ILE:CD1	2.15	0.76
1:A:29:ARG:HH11	1:A:29:ARG:CG	1.97	0.76
1:C:72:LYS:HZ1	2:C:229:2OM:H6	1.51	0.76
1:D:179:SER:HB2	1:D:192:THR:HG21	1.68	0.76
1:L:127:SER:HA	1:L:160:ARG:HH12	1.51	0.76
1:A:23:ASN:HD21	1:A:26:ASP:CG	1.88	0.76
1:J:132:GLU:HA	1:J:136:GLN:HB2	1.67	0.76
1:I:160:ARG:HB2	1:I:163:ARG:HB2	1.69	0.75
1:L:35:ARG:O	1:L:36:GLU:HG3	1.86	0.75
1:E:91:GLY:HA2	1:G:118:ARG:HH12	1.51	0.75
1:L:139:ALA:HB3	1:L:163:ARG:NH2	2.02	0.74
1:K:190:GLY:HA2	1:K:222:ILE:HD13	1.67	0.74
1:F:211:PRO:HA	1:F:214:ALA:HB3	1.68	0.74
1:E:118:ARG:HH21	1:G:118:ARG:CZ	2.01	0.73
1:H:158:SER:HB2	1:H:192:THR:OG1	1.87	0.73
1:G:189:PRO:HG2	1:G:218:ILE:HD11	1.70	0.73
1:F:219:ILE:HG12	1:F:223:LYS:HD3	1.70	0.73
1:F:9:MET:HG3	1:F:66:ARG:NH2	2.04	0.73
1:B:193:LEU:CD1	1:B:222:ILE:HG12	2.18	0.73
1:H:14:ARG:NH1	1:H:225:LEU:HD13	2.03	0.73
1:H:23:ASN:HA	1:H:51:GLU:OE2	1.89	0.73
1:F:211:PRO:HA	1:F:214:ALA:CB	2.19	0.73
1:J:163:ARG:CA	1:J:163:ARG:HH11	2.00	0.72
1:G:34:VAL:HG12	1:G:212:ALA:HA	1.71	0.72
1:F:182:VAL:HA	1:F:187:GLY:CA	2.19	0.72
1:L:201:VAL:HG13	1:L:204:SER:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:HA	1:B:163:ARG:HH11	1.54	0.72
1:L:190:GLY:HA2	1:L:225:LEU:HD21	1.72	0.72
1:J:38:ILE:HD12	1:J:38:ILE:O	1.89	0.72
1:L:171:ILE:HD11	1:L:177:LEU:HD23	1.71	0.72
1:G:82:LYS:HD3	1:H:22:MET:SD	2.30	0.71
1:J:144:ARG:O	1:J:148:ASP:HB2	1.91	0.71
1:H:14:ARG:HH11	1:H:225:LEU:HD13	1.55	0.71
1:G:113:ALA:HB1	1:G:118:ARG:O	1.91	0.71
1:C:156:GLY:O	1:C:180:PRO:HD2	1.91	0.71
1:I:133:MET:HB3	1:I:134:PHE:CD1	2.25	0.71
1:F:17:LEU:HD22	1:F:38:ILE:HG13	1.71	0.70
1:C:34:VAL:HG12	1:C:212:ALA:HA	1.70	0.70
1:M:220:GLU:OE1	1:M:223:LYS:HD3	1.92	0.70
1:B:118:ARG:NH1	1:D:60:ARG:HH12	1.89	0.70
1:H:214:ALA:O	1:H:218:ILE:HG12	1.92	0.70
1:E:29:ARG:HG2	1:E:33:GLU:OE2	1.92	0.70
1:I:22:MET:HE2	1:I:22:MET:HA	1.73	0.70
1:I:38:ILE:O	1:I:38:ILE:HD12	1.91	0.70
1:J:34:VAL:HG12	1:J:212:ALA:HA	1.73	0.70
1:G:23:ASN:HD21	1:G:26:ASP:HB2	1.56	0.69
1:K:128:HIS:HB2	1:K:129:PRO:HD2	1.74	0.69
1:G:72:LYS:HZ1	2:G:229:2OM:H6	1.58	0.69
1:B:128:HIS:HB2	1:B:129:PRO:HD2	1.75	0.69
1:F:13:ASN:O	1:F:15:LEU:N	2.26	0.69
1:F:219:ILE:HD11	1:F:223:LYS:HZ2	1.58	0.69
1:B:182:VAL:HG11	1:B:189:PRO:HG3	1.73	0.69
1:I:60:ARG:HG2	1:I:67:ILE:HD13	1.75	0.69
1:G:110:LEU:HD23	1:G:120:VAL:HG21	1.75	0.69
1:F:15:LEU:HD11	1:F:201:VAL:HG23	1.74	0.69
1:L:166:ARG:HH11	1:L:166:ARG:HG3	1.58	0.69
1:D:164:LEU:HD21	1:D:192:THR:HG23	1.75	0.68
1:J:209:ASP:O	1:J:211:PRO:HD3	1.94	0.68
1:K:72:LYS:HB3	1:K:98:HIS:CD2	2.28	0.68
1:E:29:ARG:O	1:E:33:GLU:HG3	1.93	0.68
1:D:129:PRO:O	1:D:132:GLU:HG2	1.93	0.68
1:H:37:TYR:HB3	1:H:219:ILE:HD11	1.74	0.68
1:M:10:ASP:OD2	1:M:11:VAL:O	2.09	0.68
1:L:142:ILE:HG23	1:L:145:MET:HE2	1.76	0.68
1:G:203:ARG:HB3	1:G:207:LEU:HD12	1.75	0.68
1:E:182:VAL:HG21	1:E:199:ILE:HB	1.75	0.68
1:M:210:ASN:ND2	1:M:213:ALA:HB2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:VAL:HG21	1:E:218:ILE:HD13	1.75	0.68
1:L:139:ALA:HB3	1:L:163:ARG:HH21	1.59	0.68
1:D:205:ILE:HD11	1:D:218:ILE:HD12	1.74	0.68
1:I:48:VAL:HG11	1:I:53:MET:SD	2.34	0.68
1:A:29:ARG:O	1:A:33:GLU:HG3	1.95	0.67
1:D:72:LYS:HZ1	2:D:229:2OM:H6	1.59	0.67
1:F:21:LEU:HD12	1:F:27:ALA:HA	1.77	0.67
1:B:156:GLY:O	1:B:180:PRO:HD2	1.93	0.67
1:M:219:ILE:O	1:M:223:LYS:HG3	1.94	0.67
1:E:104:ASP:OD2	1:F:129:PRO:HG2	1.95	0.67
1:J:102:GLY:O	1:J:106:VAL:HG23	1.95	0.66
1:I:165:SER:HA	1:I:195:PHE:CD2	2.30	0.66
1:E:37:TYR:HB3	1:E:219:ILE:HD11	1.76	0.66
1:L:35:ARG:HD3	1:L:63:PHE:HB3	1.78	0.66
1:G:163:ARG:NH2	1:G:167:LEU:HD21	2.11	0.66
1:G:165:SER:HB2	1:G:195:PHE:CE1	2.30	0.66
1:E:40:THR:HG23	1:E:66:ARG:HB2	1.77	0.66
1:E:129:PRO:HG2	1:F:104:ASP:OD2	1.96	0.66
1:H:201:VAL:HG11	1:H:205:ILE:HD13	1.79	0.66
1:B:219:ILE:O	1:B:223:LYS:HB2	1.95	0.66
1:B:182:VAL:CG1	1:B:189:PRO:HG3	2.25	0.65
1:E:132:GLU:HA	1:E:136:GLN:HB2	1.76	0.65
1:L:177:LEU:CD1	1:L:196:ALA:HA	2.27	0.65
1:J:37:TYR:CZ	1:J:216:ALA:HB2	2.32	0.65
1:I:142:ILE:HG23	1:I:145:MET:HE2	1.77	0.65
1:K:108:ALA:O	1:K:112:VAL:HG23	1.97	0.65
1:I:188:ASP:HB2	1:I:189:PRO:HD2	1.78	0.65
1:I:190:GLY:HA2	1:I:225:LEU:HD22	1.77	0.65
1:J:182:VAL:HG11	1:J:189:PRO:HG3	1.78	0.65
1:E:78:GLU:HG2	1:F:203:ARG:HH12	1.59	0.65
1:B:118:ARG:CZ	1:D:60:ARG:HH12	2.10	0.64
1:J:205:ILE:HD11	1:J:218:ILE:HD12	1.78	0.64
1:H:16:ILE:HB	1:H:200:ILE:HG23	1.80	0.64
1:A:104:ASP:OD2	1:B:129:PRO:HG2	1.97	0.64
1:E:178:ILE:HD12	1:E:200:ILE:HD11	1.79	0.64
1:D:37:TYR:CE2	1:D:216:ALA:HB2	2.32	0.64
1:A:158:SER:HB2	1:A:192:THR:OG1	1.97	0.64
1:L:21:LEU:HD11	1:L:206:TYR:HB2	1.80	0.64
1:F:52:GLY:O	1:F:55:ILE:HG22	1.97	0.64
1:I:141:GLU:HB3	1:J:134:PHE:HE2	1.61	0.64
1:B:29:ARG:HD2	1:B:33:GLU:OE1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:10:ASP:OD2	1:M:11:VAL:N	2.31	0.64
1:H:72:LYS:HZ1	2:H:229:2OM:H6	1.62	0.64
1:F:157:PRO:O	1:F:164:LEU:HD13	1.96	0.64
1:K:62:ARG:HB3	1:K:62:ARG:NH1	2.13	0.64
1:E:34:VAL:HG12	1:E:212:ALA:HA	1.80	0.64
1:D:139:ALA:HB3	1:D:163:ARG:NH2	2.13	0.64
1:K:193:LEU:CD1	1:K:222:ILE:HG12	2.23	0.63
1:E:61:LYS:HD2	1:G:9:MET:CA	2.25	0.63
1:F:182:VAL:CG2	1:F:201:VAL:HG22	2.29	0.63
1:F:138:ALA:O	1:F:142:ILE:HG13	1.97	0.63
1:D:88:PHE:O	1:D:91:GLY:N	2.27	0.63
1:A:60:ARG:HB2	1:A:67:ILE:HD12	1.81	0.63
1:B:160:ARG:HB3	1:B:163:ARG:HG2	1.79	0.63
1:L:37:TYR:HB3	1:L:219:ILE:HD11	1.79	0.63
1:E:85:ARG:HA	1:E:116:MET:HE3	1.80	0.63
1:H:98:HIS:CE1	1:H:123:LEU:HD23	2.33	0.63
1:L:177:LEU:HD11	1:L:196:ALA:HA	1.81	0.63
1:F:15:LEU:CD1	1:F:201:VAL:HG23	2.28	0.63
1:C:78:GLU:HG2	1:D:203:ARG:HH12	1.64	0.63
1:L:168:ARG:CG	1:L:173:GLN:HE22	2.04	0.62
1:J:210:ASN:ND2	1:J:213:ALA:HB2	2.10	0.62
1:K:148:ASP:HB3	1:K:149:LEU:HD22	1.80	0.62
1:F:19:MET:HE1	1:F:30:VAL:HB	1.80	0.62
1:L:180:PRO:HB3	1:L:200:ILE:HD12	1.80	0.62
1:L:214:ALA:O	1:L:218:ILE:HG13	2.00	0.62
1:E:165:SER:HB2	1:E:195:PHE:CE1	2.35	0.62
1:I:220:GLU:O	1:I:223:LYS:HB2	1.98	0.62
1:E:72:LYS:HZ1	2:E:229:2OM:H6	1.63	0.62
1:K:102:GLY:O	1:K:106:VAL:HG23	2.00	0.62
1:F:205:ILE:O	1:F:211:PRO:HB3	2.00	0.62
1:G:220:GLU:OE2	1:G:223:LYS:HD2	1.98	0.62
1:L:72:LYS:HZ1	2:L:229:2OM:H6	1.64	0.62
1:E:113:ALA:HB1	1:E:118:ARG:O	1.99	0.62
1:H:201:VAL:CG1	1:H:205:ILE:HD13	2.30	0.62
1:D:184:ALA:HB2	1:D:203:ARG:HB2	1.80	0.62
1:K:163:ARG:HA	1:K:163:ARG:HH11	1.65	0.61
1:K:26:ASP:HA	1:K:29:ARG:NH1	2.13	0.61
1:C:37:TYR:HB3	1:C:219:ILE:HD11	1.81	0.61
1:D:24:ARG:HB2	1:D:51:GLU:OE2	1.99	0.61
1:G:24:ARG:HB2	1:G:51:GLU:CD	2.21	0.61
1:L:38:ILE:C	1:L:38:ILE:HD12	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:ILE:HG12	1:H:100:PHE:CE2	2.35	0.61
1:C:178:ILE:HD12	1:C:200:ILE:HD11	1.80	0.61
1:K:158:SER:HB3	1:K:180:PRO:O	2.00	0.61
1:K:145:MET:O	1:K:149:LEU:HD23	2.00	0.61
1:B:205:ILE:HD13	1:B:215:ALA:HB2	1.82	0.61
1:I:36:GLU:HG3	1:I:37:TYR:CE1	2.36	0.61
1:K:167:LEU:O	1:K:171:ILE:HG12	2.01	0.61
1:F:66:ARG:HA	1:F:93:ASP:OD2	2.01	0.61
1:F:219:ILE:HD11	1:F:223:LYS:HZ3	1.63	0.61
1:F:15:LEU:HD12	1:F:16:ILE:H	1.65	0.61
1:K:104:ASP:OD1	1:L:130:GLY:HA3	2.01	0.61
1:E:53:MET:SD	1:F:49:LEU:HD22	2.41	0.61
1:L:29:ARG:O	1:L:33:GLU:HG3	2.00	0.60
1:F:144:ARG:O	1:F:147:VAL:HB	2.01	0.60
1:B:55:ILE:O	1:B:59:PHE:HD1	1.83	0.60
1:B:30:VAL:HG11	1:B:206:TYR:HA	1.81	0.60
1:F:15:LEU:HD12	1:F:199:ILE:O	2.02	0.60
1:K:131:ALA:HB3	1:K:160:ARG:HH22	1.66	0.60
1:D:85:ARG:HH12	1:D:115:GLU:CD	2.03	0.60
1:K:111:ASN:O	1:K:115:GLU:HG3	2.00	0.60
1:K:182:VAL:HG21	1:K:199:ILE:HB	1.83	0.60
1:B:118:ARG:NH1	1:D:60:ARG:NH1	2.49	0.60
1:F:219:ILE:O	1:F:223:LYS:HB2	2.01	0.60
1:G:218:ILE:O	1:G:221:SER:HB3	2.00	0.60
1:D:139:ALA:HB3	1:D:163:ARG:HH21	1.67	0.60
1:A:29:ARG:CG	1:A:29:ARG:NH1	2.61	0.60
1:E:61:LYS:O	1:G:10:ASP:HB3	2.02	0.60
1:D:11:VAL:HG12	1:D:40:THR:OG1	2.01	0.60
1:D:220:GLU:HA	1:D:223:LYS:HD3	1.82	0.60
1:I:182:VAL:HG12	1:I:183:GLY:N	2.17	0.60
1:I:220:GLU:HA	1:I:223:LYS:HE3	1.83	0.60
1:K:135:ILE:HD11	1:L:101:PRO:HA	1.83	0.60
1:E:224:ASP:OD2	1:E:225:LEU:HD12	2.01	0.60
1:D:219:ILE:O	1:D:223:LYS:HG3	2.01	0.60
1:A:189:PRO:HB3	1:A:222:ILE:HD11	1.84	0.60
1:A:72:LYS:HZ1	2:A:229:2OM:H6	1.67	0.60
1:E:23:ASN:ND2	1:E:26:ASP:H	1.99	0.59
1:D:163:ARG:HB3	1:D:163:ARG:NH1	2.17	0.59
1:K:190:GLY:HA2	1:K:222:ILE:CD1	2.32	0.59
1:L:98:HIS:CE1	1:L:123:LEU:HD23	2.37	0.59
1:K:21:LEU:HD13	1:K:26:ASP:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:163:ARG:O	1:H:167:LEU:HG	2.02	0.59
1:I:177:LEU:HD23	1:I:196:ALA:HA	1.82	0.59
1:J:163:ARG:NH1	1:J:163:ARG:HA	2.07	0.59
1:D:203:ARG:HG3	1:D:206:TYR:OH	2.03	0.59
1:F:163:ARG:HB3	1:F:163:ARG:NH1	2.17	0.59
1:M:37:TYR:HB3	1:M:219:ILE:HD11	1.83	0.59
1:I:190:GLY:HA2	1:I:225:LEU:CD2	2.33	0.59
1:L:180:PRO:O	1:L:182:VAL:N	2.35	0.59
1:H:81:GLU:HG2	1:H:85:ARG:NH2	2.18	0.59
1:E:23:ASN:HD21	1:E:26:ASP:CG	2.06	0.59
1:E:138:ALA:O	1:E:142:ILE:HG13	2.03	0.59
1:L:153:ASN:HA	1:L:176:PHE:O	2.02	0.59
1:E:88:PHE:O	1:E:91:GLY:N	2.32	0.59
1:K:149:LEU:HD22	1:K:149:LEU:N	2.17	0.59
1:L:166:ARG:O	1:L:170:ILE:HG13	2.02	0.59
1:F:162:GLU:HG2	1:F:163:ARG:N	2.18	0.58
1:H:160:ARG:HD3	1:H:163:ARG:HG3	1.84	0.58
1:K:72:LYS:HZ1	2:K:229:2OM:H6	1.69	0.58
1:B:29:ARG:HH11	1:B:29:ARG:HG3	1.68	0.58
1:C:37:TYR:CZ	1:C:216:ALA:HB2	2.38	0.58
1:B:31:THR:HG21	1:B:59:PHE:HE2	1.69	0.58
1:L:28:LEU:HD13	1:L:62:ARG:NH1	2.19	0.58
1:L:201:VAL:CG1	1:L:204:SER:HB3	2.34	0.58
1:M:117:GLY:O	1:M:118:ARG:NH1	2.35	0.58
1:F:72:LYS:HZ1	2:F:229:2OM:H6	1.68	0.58
1:H:215:ALA:O	1:H:219:ILE:HG13	2.03	0.58
1:D:110:LEU:O	1:D:114:GLU:HB2	2.03	0.58
1:G:132:GLU:HG2	1:G:136:GLN:OE1	2.04	0.58
1:K:17:LEU:HD22	1:K:34:VAL:HG21	1.84	0.58
1:F:12:MET:HB3	1:F:38:ILE:HA	1.86	0.58
1:K:117:GLY:O	1:K:118:ARG:HD3	2.03	0.58
1:K:162:GLU:HG2	1:K:163:ARG:N	2.19	0.58
1:D:163:ARG:HA	1:D:163:ARG:HH11	1.68	0.58
1:K:32:GLY:HA2	1:K:63:PHE:HE2	1.69	0.58
1:E:224:ASP:CG	1:E:225:LEU:HD12	2.23	0.58
1:F:193:LEU:CD2	1:F:222:ILE:HG12	2.32	0.58
1:L:142:ILE:O	1:L:145:MET:HB3	2.04	0.58
1:F:128:HIS:HB2	1:F:129:PRO:HD2	1.86	0.58
1:M:156:GLY:O	1:M:180:PRO:HD2	2.03	0.58
1:I:182:VAL:HG12	1:I:183:GLY:H	1.69	0.58
1:G:34:VAL:O	1:G:38:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:158:SER:HB2	1:K:179:SER:OG	2.04	0.58
1:F:163:ARG:O	1:F:167:LEU:HG	2.03	0.57
1:D:164:LEU:CD2	1:D:192:THR:HG23	2.34	0.57
1:I:140:ASP:O	1:I:144:ARG:HG3	2.03	0.57
1:F:164:LEU:HD23	1:F:195:PHE:HE1	1.68	0.57
1:J:66:ARG:HH11	1:J:66:ARG:CB	2.16	0.57
1:C:203:ARG:NH1	1:D:78:GLU:HG2	2.19	0.57
1:C:24:ARG:HH11	1:C:24:ARG:HG2	1.68	0.57
1:G:166:ARG:O	1:G:170:ILE:HG13	2.05	0.57
1:F:178:ILE:HA	1:F:198:ALA:O	2.03	0.57
1:G:41:VAL:HG12	1:G:43:ILE:HD13	1.87	0.57
1:G:210:ASN:ND2	1:G:213:ALA:H	2.03	0.57
1:L:182:VAL:HG13	1:L:187:GLY:O	2.04	0.57
1:C:162:GLU:OE2	1:C:162:GLU:N	2.32	0.57
1:D:201:VAL:HG13	1:D:204:SER:HB2	1.87	0.57
1:F:34:VAL:HG13	1:F:212:ALA:HA	1.87	0.57
1:B:161:PRO:HB3	1:B:191:GLU:OE1	2.05	0.57
1:D:206:TYR:CE1	1:D:207:LEU:HG	2.40	0.57
1:G:42:LYS:O	1:G:43:ILE:HD12	2.05	0.56
1:K:38:ILE:C	1:K:38:ILE:HD12	2.26	0.56
1:B:35:ARG:O	1:B:35:ARG:NH1	2.38	0.56
1:I:157:PRO:O	1:I:164:LEU:HD21	2.06	0.56
1:D:72:LYS:NZ	2:D:229:2OM:H6	2.19	0.56
1:E:9:MET:CE	1:E:66:ARG:HH21	2.17	0.56
1:L:206:TYR:CE1	1:L:207:LEU:HG	2.40	0.56
1:L:56:ILE:HD12	1:L:67:ILE:HG21	1.88	0.56
1:L:113:ALA:HB1	1:L:118:ARG:O	2.06	0.56
1:E:21:LEU:HD12	1:E:27:ALA:HA	1.88	0.56
1:G:33:GLU:O	1:G:212:ALA:HB2	2.06	0.56
1:C:214:ALA:O	1:C:218:ILE:HG13	2.04	0.56
1:H:30:VAL:O	1:H:34:VAL:HG22	2.05	0.56
1:B:129:PRO:O	1:B:132:GLU:HG3	2.05	0.56
1:B:72:LYS:HZ1	2:B:229:2OM:H6	1.70	0.56
1:B:66:ARG:NH2	1:D:64:GLY:O	2.38	0.56
1:E:42:LYS:NZ	1:E:70:ASP:OD2	2.33	0.56
1:F:152:LYS:NZ	1:F:152:LYS:HB3	2.19	0.56
1:F:155:VAL:HG22	1:F:178:ILE:HD11	1.88	0.56
1:E:60:ARG:O	1:E:64:GLY:N	2.38	0.56
1:E:125:GLU:O	1:E:157:PRO:HD3	2.05	0.56
1:L:177:LEU:HD11	1:L:195:PHE:O	2.06	0.56
1:B:222:ILE:HD11	1:B:225:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:ARG:CG	1:I:67:ILE:HD13	2.35	0.56
1:B:29:ARG:O	1:B:32:GLY:N	2.39	0.56
1:I:129:PRO:HB2	1:J:104:ASP:OD2	2.06	0.56
1:H:45:TYR:N	1:H:46:PRO:CD	2.69	0.56
1:K:24:ARG:CZ	1:K:24:ARG:HB3	2.36	0.56
1:C:37:TYR:HB3	1:C:219:ILE:CD1	2.35	0.56
1:K:21:LEU:HD12	1:K:27:ALA:HA	1.88	0.55
1:K:166:ARG:HG3	1:K:166:ARG:HH11	1.70	0.55
1:B:201:VAL:CG1	1:B:204:SER:HB2	2.36	0.55
1:F:38:ILE:HD13	1:F:38:ILE:N	2.21	0.55
1:K:178:ILE:HD12	1:K:200:ILE:HD11	1.88	0.55
1:C:210:ASN:HB3	1:C:213:ALA:HB3	1.89	0.55
1:F:37:TYR:OH	1:F:216:ALA:HB2	2.06	0.55
1:D:38:ILE:HD12	1:D:40:THR:N	2.20	0.55
1:D:162:GLU:HG2	1:D:163:ARG:N	2.21	0.55
1:D:191:GLU:O	1:D:194:ARG:HG3	2.06	0.55
1:F:17:LEU:N	1:F:17:LEU:HD23	2.22	0.55
1:I:158:SER:N	1:I:179:SER:HB2	2.20	0.55
1:G:23:ASN:ND2	1:G:26:ASP:HB2	2.21	0.55
1:G:120:VAL:HG23	1:G:120:VAL:O	2.05	0.55
1:G:41:VAL:HG12	1:G:43:ILE:CD1	2.36	0.55
1:M:107:ARG:NH2	1:M:149:LEU:CD2	2.69	0.55
1:G:180:PRO:HG3	2:G:229:2OM:O71	2.06	0.55
1:I:177:LEU:HD23	1:I:195:PHE:O	2.06	0.55
1:C:118:ARG:NH2	1:F:118:ARG:CZ	2.70	0.55
1:F:221:SER:O	1:F:222:ILE:HG23	2.07	0.54
1:G:215:ALA:O	1:G:218:ILE:HG22	2.07	0.54
1:M:10:ASP:OD2	1:M:11:VAL:C	2.46	0.54
1:E:108:ALA:O	1:E:112:VAL:HG23	2.07	0.54
1:E:124:THR:OG1	1:E:167:LEU:HD13	2.05	0.54
1:L:160:ARG:O	1:L:163:ARG:HB2	2.07	0.54
1:K:210:ASN:O	1:K:213:ALA:HB3	2.07	0.54
1:L:39:ASP:O	1:L:65:CYS:HB2	2.07	0.54
1:J:62:ARG:HG2	1:J:62:ARG:HH11	1.72	0.54
1:B:190:GLY:HA2	1:B:222:ILE:HD13	1.89	0.54
1:D:158:SER:OG	1:D:182:VAL:HG22	2.08	0.54
1:A:73:VAL:HB	1:A:97:VAL:HG22	1.89	0.54
1:J:220:GLU:C	1:J:222:ILE:H	2.11	0.54
1:H:19:MET:HG3	1:H:47:LEU:CD2	2.37	0.54
1:I:166:ARG:O	1:I:166:ARG:HD2	2.08	0.54
1:K:125:GLU:HA	1:K:135:ILE:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:215:ALA:O	1:K:219:ILE:HG13	2.06	0.54
1:G:14:ARG:HH21	1:G:193:LEU:HB3	1.72	0.54
1:G:21:LEU:HD12	1:G:27:ALA:HA	1.90	0.53
1:I:36:GLU:HG3	1:I:37:TYR:CD1	2.43	0.53
1:E:162:GLU:OE2	1:E:162:GLU:N	2.34	0.53
1:C:38:ILE:C	1:C:38:ILE:HD12	2.28	0.53
1:I:101:PRO:O	1:J:128:HIS:NE2	2.37	0.53
1:E:23:ASN:OD1	1:E:26:ASP:HB2	2.08	0.53
1:G:88:PHE:O	1:G:91:GLY:N	2.37	0.53
1:E:201:VAL:CG1	1:E:204:SER:HB2	2.39	0.53
1:L:151:VAL:HG12	1:L:153:ASN:H	1.73	0.53
1:G:49:LEU:HD21	1:H:45:TYR:HE2	1.73	0.53
1:E:210:ASN:HB3	1:E:213:ALA:HB3	1.90	0.53
1:K:180:PRO:HG3	2:K:229:2OM:O71	2.09	0.53
1:H:13:ASN:ND2	1:H:219:ILE:HD13	2.24	0.53
1:K:138:ALA:O	1:K:142:ILE:HG13	2.09	0.53
1:G:47:LEU:O	1:G:51:GLU:HB2	2.08	0.53
1:K:183:GLY:HA3	1:K:204:SER:OG	2.09	0.53
1:D:163:ARG:HB3	1:D:163:ARG:CZ	2.37	0.53
1:K:122:LEU:HD12	1:K:123:LEU:N	2.24	0.53
1:D:14:ARG:HH21	1:D:193:LEU:HG	1.73	0.53
1:A:12:MET:HB2	1:A:39:ASP:CG	2.29	0.53
1:K:66:ARG:HG3	1:K:66:ARG:HH11	1.73	0.53
1:F:38:ILE:HD13	1:F:38:ILE:H	1.74	0.52
1:E:222:ILE:HG23	1:E:225:LEU:HD22	1.90	0.52
1:B:28:LEU:HD23	1:B:63:PHE:HE1	1.73	0.52
1:K:23:ASN:HA	1:K:51:GLU:OE2	2.10	0.52
1:L:138:ALA:HB1	1:L:141:GLU:HB3	1.91	0.52
1:M:9:MET:O	1:M:9:MET:CG	2.56	0.52
1:B:191:GLU:HA	1:B:194:ARG:HD3	1.91	0.52
1:M:152:LYS:NZ	1:M:152:LYS:HB3	2.24	0.52
1:B:222:ILE:HG13	1:B:222:ILE:O	2.09	0.52
1:D:26:ASP:O	1:D:30:VAL:HG23	2.10	0.52
1:H:81:GLU:HG3	1:H:112:VAL:HG23	1.92	0.52
1:I:46:PRO:HB2	3:I:234:HOH:O	2.08	0.52
1:I:34:VAL:O	1:I:34:VAL:HG22	2.10	0.52
1:F:97:VAL:HG12	1:F:98:HIS:O	2.10	0.52
1:E:37:TYR:CZ	1:E:216:ALA:HB2	2.45	0.52
1:H:192:THR:CG2	1:H:199:ILE:HG22	2.40	0.52
1:L:219:ILE:HA	1:L:222:ILE:HD12	1.92	0.52
1:G:184:ALA:HB1	1:G:203:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:142:ILE:O	1:K:145:MET:HB3	2.10	0.52
1:B:28:LEU:O	1:B:63:PHE:HZ	1.93	0.52
1:I:35:ARG:HD3	1:I:63:PHE:HB3	1.92	0.52
1:E:52:GLY:O	1:E:55:ILE:HG22	2.10	0.52
1:D:155:VAL:HG22	1:D:178:ILE:HD11	1.92	0.52
1:L:26:ASP:O	1:L:30:VAL:HG23	2.10	0.52
1:F:30:VAL:O	1:F:34:VAL:HG22	2.10	0.52
1:K:102:GLY:HA3	1:L:130:GLY:O	2.09	0.52
1:I:35:ARG:O	1:I:35:ARG:HG3	2.09	0.52
1:L:35:ARG:C	1:L:36:GLU:HG3	2.30	0.52
1:F:14:ARG:HG2	1:F:197:ASP:O	2.10	0.52
1:F:100:PHE:N	1:F:101:PRO:CD	2.73	0.52
1:B:62:ARG:HG3	1:B:62:ARG:HH11	1.75	0.52
1:L:223:LYS:NZ	1:L:223:LYS:HA	2.25	0.52
1:J:98:HIS:CE1	1:J:123:LEU:HD23	2.45	0.51
1:L:193:LEU:HB2	1:L:225:LEU:HD11	1.91	0.51
1:G:167:LEU:O	1:G:171:ILE:HG12	2.10	0.51
1:E:177:LEU:HD12	1:E:178:ILE:N	2.25	0.51
1:G:14:ARG:HG2	1:G:197:ASP:O	2.10	0.51
1:A:104:ASP:OD1	1:B:130:GLY:HA3	2.11	0.51
1:L:166:ARG:NH1	1:L:166:ARG:HG3	2.25	0.51
1:B:206:TYR:CD1	1:B:207:LEU:HG	2.45	0.51
1:G:135:ILE:HG12	1:H:100:PHE:CD2	2.45	0.51
1:I:222:ILE:O	1:I:222:ILE:HG22	2.09	0.51
1:H:143:ALA:O	1:H:147:VAL:HG23	2.09	0.51
1:K:205:ILE:HD11	1:K:218:ILE:HD12	1.91	0.51
1:A:37:TYR:HB3	1:A:219:ILE:CD1	2.40	0.51
1:I:183:GLY:O	1:I:203:ARG:HD2	2.09	0.51
1:E:49:LEU:HD22	1:F:53:MET:CE	2.40	0.51
1:K:87:THR:HG21	1:K:95:ILE:HD12	1.91	0.51
1:G:117:GLY:O	1:G:118:ARG:HD2	2.10	0.51
1:L:183:GLY:O	1:L:184:ALA:HB2	2.10	0.51
1:L:206:TYR:CD1	1:L:207:LEU:HG	2.46	0.51
1:C:130:GLY:HA3	1:D:104:ASP:OD1	2.10	0.51
1:K:29:ARG:NH1	1:K:29:ARG:HB3	2.26	0.51
1:L:72:LYS:NZ	2:L:229:2OM:H6	2.24	0.51
1:L:223:LYS:HA	1:L:223:LYS:HZ3	1.75	0.51
1:J:120:VAL:O	1:J:153:ASN:HB2	2.11	0.51
1:I:52:GLY:O	1:I:55:ILE:HG22	2.11	0.51
1:K:129:PRO:O	1:K:131:ALA:N	2.44	0.51
1:A:192:THR:HG21	1:A:199:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:166:ARG:O	1:M:169:GLU:HG2	2.10	0.51
1:K:49:LEU:HD22	1:L:53:MET:SD	2.50	0.51
1:E:156:GLY:O	1:E:180:PRO:HD2	2.11	0.51
1:F:200:ILE:N	1:F:200:ILE:HD12	2.26	0.51
1:B:215:ALA:O	1:B:219:ILE:HD13	2.09	0.51
1:E:136:GLN:HA	1:E:136:GLN:HE21	1.76	0.51
1:G:210:ASN:HD22	1:G:213:ALA:HB3	1.76	0.51
1:B:19:MET:HE3	1:B:21:LEU:HD12	1.93	0.51
1:E:61:LYS:CD	1:G:9:MET:HA	2.35	0.51
1:E:118:ARG:HH21	1:G:118:ARG:NE	2.09	0.51
1:G:107:ARG:HH21	1:G:149:LEU:HD13	1.76	0.51
1:F:21:LEU:HD21	1:F:206:TYR:HB2	1.93	0.51
1:K:107:ARG:HE	1:K:149:LEU:HD12	1.76	0.51
1:G:220:GLU:HA	1:G:223:LYS:HB2	1.93	0.51
1:K:32:GLY:HA2	1:K:63:PHE:CE2	2.45	0.51
1:E:203:ARG:NH1	1:F:78:GLU:HG2	2.25	0.51
1:B:14:ARG:O	1:B:198:ALA:HB1	2.10	0.51
1:A:81:GLU:HG3	1:A:112:VAL:CG2	2.41	0.51
1:D:180:PRO:HB3	1:D:200:ILE:HD12	1.93	0.50
1:B:62:ARG:HG3	1:B:62:ARG:O	2.11	0.50
1:F:125:GLU:HG2	1:F:157:PRO:HG3	1.93	0.50
1:E:104:ASP:OD1	1:F:130:GLY:HA3	2.10	0.50
1:D:58:GLU:O	1:D:62:ARG:HB2	2.10	0.50
1:H:113:ALA:HB2	1:H:120:VAL:HG23	1.92	0.50
1:I:158:SER:HB2	1:I:192:THR:CG2	2.41	0.50
1:E:222:ILE:CG2	1:E:225:LEU:HD22	2.41	0.50
1:G:164:LEU:HG	1:G:195:PHE:HB2	1.93	0.50
1:I:205:ILE:HD11	1:I:218:ILE:HD12	1.93	0.50
1:M:38:ILE:C	1:M:38:ILE:HD12	2.32	0.50
1:D:183:GLY:HA3	1:D:204:SER:OG	2.11	0.50
1:E:120:VAL:O	1:E:153:ASN:HB2	2.10	0.50
1:L:37:TYR:CD1	1:L:37:TYR:N	2.80	0.50
1:I:48:VAL:CG1	1:I:53:MET:SD	2.99	0.50
1:I:158:SER:HB2	1:I:192:THR:HG21	1.93	0.50
1:K:100:PHE:N	1:K:101:PRO:HD2	2.27	0.50
1:F:199:ILE:C	1:F:200:ILE:HD12	2.32	0.50
1:F:37:TYR:CZ	1:F:216:ALA:HB2	2.47	0.50
1:L:184:ALA:CB	1:L:203:ARG:HE	2.25	0.50
1:G:180:PRO:HD3	1:G:200:ILE:HD12	1.93	0.50
1:F:34:VAL:CG1	1:F:212:ALA:HA	2.42	0.50
1:E:19:MET:HG3	1:E:47:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLY:HA3	1:D:89:LYS:O	2.11	0.50
1:E:171:ILE:HD12	1:E:172:GLY:N	2.26	0.50
1:A:24:ARG:NH2	1:A:58:GLU:OE2	2.45	0.50
1:A:7:ASP:O	1:J:61:LYS:HD2	2.11	0.50
1:G:115:GLU:HG2	1:G:115:GLU:O	2.10	0.50
1:F:123:LEU:HD12	1:F:155:VAL:HB	1.93	0.49
1:F:143:ALA:O	1:F:147:VAL:HG23	2.12	0.49
1:K:182:VAL:HG13	1:K:187:GLY:O	2.11	0.49
1:C:113:ALA:HB1	1:C:118:ARG:O	2.10	0.49
1:A:143:ALA:O	1:A:147:VAL:HG23	2.12	0.49
1:F:163:ARG:HB3	1:F:163:ARG:HH11	1.75	0.49
1:E:206:TYR:CD1	1:E:207:LEU:HG	2.47	0.49
1:H:210:ASN:HD22	1:H:213:ALA:CB	2.17	0.49
1:I:184:ALA:HB3	1:I:185:GLN:NE2	2.27	0.49
1:M:107:ARG:NH2	1:M:149:LEU:HD23	2.28	0.49
1:D:29:ARG:HG2	1:D:33:GLU:OE2	2.13	0.49
1:I:14:ARG:HD2	1:I:193:LEU:HD22	1.94	0.49
1:G:37:TYR:HB3	1:G:219:ILE:HD11	1.94	0.49
1:L:125:GLU:HB3	1:L:157:PRO:HD3	1.93	0.49
1:C:104:ASP:N	1:C:104:ASP:OD1	2.46	0.49
1:E:37:TYR:HB3	1:E:219:ILE:HD12	1.92	0.49
1:H:37:TYR:CE1	1:H:216:ALA:HB2	2.47	0.49
1:I:216:ALA:O	1:I:220:GLU:HB2	2.13	0.49
1:F:136:GLN:HG3	1:F:163:ARG:HH21	1.77	0.49
1:C:78:GLU:HG2	1:D:203:ARG:NH1	2.27	0.49
1:G:12:MET:HB2	1:G:39:ASP:OD1	2.13	0.49
1:L:177:LEU:HD12	1:L:177:LEU:C	2.33	0.49
1:G:205:ILE:HD13	1:G:215:ALA:HB2	1.93	0.49
1:L:180:PRO:HA	1:L:200:ILE:HB	1.95	0.49
1:H:81:GLU:HG2	1:H:85:ARG:HH21	1.76	0.49
1:I:128:HIS:HB2	1:I:129:PRO:HD2	1.95	0.49
1:F:41:VAL:HB	1:F:67:ILE:HD13	1.95	0.49
1:I:58:GLU:HG2	1:I:62:ARG:HD2	1.95	0.49
1:E:118:ARG:HH21	1:G:118:ARG:NH2	2.10	0.49
1:D:219:ILE:HG22	1:D:223:LYS:HG3	1.94	0.49
1:L:25:ASP:O	1:L:29:ARG:HB2	2.13	0.49
1:I:183:GLY:O	1:I:184:ALA:HB2	2.13	0.49
1:I:15:LEU:O	1:I:38:ILE:HG22	2.13	0.49
1:K:112:VAL:HG12	1:K:116:MET:CE	2.43	0.49
1:K:152:LYS:HB3	1:K:152:LYS:HZ3	1.77	0.49
1:B:210:ASN:HD21	1:B:212:ALA:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:138:ALA:O	1:J:142:ILE:HG13	2.13	0.48
1:D:214:ALA:O	1:D:218:ILE:HG13	2.12	0.48
1:D:29:ARG:O	1:D:33:GLU:HG3	2.13	0.48
1:D:164:LEU:O	1:D:167:LEU:HB3	2.13	0.48
1:K:85:ARG:HA	1:K:116:MET:HE1	1.94	0.48
1:K:37:TYR:HB3	1:K:219:ILE:CD1	2.43	0.48
1:M:178:ILE:HD12	1:M:200:ILE:HD11	1.95	0.48
1:F:35:ARG:NH1	1:F:35:ARG:O	2.43	0.48
1:F:39:ASP:O	1:F:66:ARG:HG2	2.13	0.48
1:F:17:LEU:N	1:F:17:LEU:CD2	2.77	0.48
1:L:219:ILE:O	1:L:222:ILE:HB	2.13	0.48
1:G:17:LEU:HB3	1:G:38:ILE:HD12	1.94	0.48
1:J:37:TYR:HE1	1:J:212:ALA:O	1.96	0.48
1:I:220:GLU:HG3	1:I:223:LYS:NZ	2.28	0.48
1:C:24:ARG:NH1	1:C:24:ARG:HG2	2.28	0.48
1:B:191:GLU:O	1:B:194:ARG:HD3	2.13	0.48
1:A:130:GLY:HA3	1:B:104:ASP:OD1	2.12	0.48
1:B:45:TYR:N	1:B:46:PRO:CD	2.75	0.48
1:E:223:LYS:O	1:E:224:ASP:HB3	2.13	0.48
1:B:193:LEU:HD12	1:B:222:ILE:CG1	2.39	0.48
1:D:167:LEU:HD13	1:D:167:LEU:C	2.34	0.48
1:H:36:GLU:HG3	1:H:37:TYR:CD2	2.47	0.48
1:D:201:VAL:CG1	1:D:204:SER:HB2	2.43	0.48
1:G:177:LEU:HD23	1:G:195:PHE:O	2.13	0.48
1:E:48:VAL:HG11	1:E:53:MET:SD	2.53	0.48
1:A:24:ARG:HG2	1:A:24:ARG:HH11	1.77	0.48
1:D:208:ALA:O	1:D:209:ASP:C	2.51	0.48
1:F:98:HIS:CE1	1:F:123:LEU:HD23	2.49	0.48
1:M:9:MET:HB2	1:M:66:ARG:HH21	1.78	0.48
1:F:19:MET:HE3	1:F:31:THR:OG1	2.14	0.48
1:K:49:LEU:O	1:L:53:MET:HG3	2.13	0.48
1:F:213:ALA:HA	1:F:216:ALA:HB3	1.94	0.48
1:G:85:ARG:HH11	1:G:85:ARG:HG3	1.79	0.48
1:B:136:GLN:HE21	1:B:163:ARG:NE	1.91	0.48
1:A:104:ASP:OD2	1:B:130:GLY:N	2.36	0.48
1:K:14:ARG:HH12	1:K:225:LEU:HD23	1.79	0.48
1:D:179:SER:CB	1:D:192:THR:HG21	2.42	0.48
1:L:218:ILE:O	1:L:222:ILE:HG13	2.13	0.48
1:G:34:VAL:C	1:G:36:GLU:N	2.67	0.48
1:D:162:GLU:HG2	1:D:163:ARG:H	1.79	0.48
1:H:81:GLU:HG3	1:H:112:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:ALA:HB1	1:I:118:ARG:O	2.14	0.48
1:C:124:THR:HG21	1:C:167:LEU:HD21	1.96	0.48
1:G:124:THR:HG22	1:G:142:ILE:HG22	1.96	0.48
1:J:38:ILE:HD12	1:J:38:ILE:C	2.33	0.48
1:I:176:PHE:HA	1:I:197:ASP:OD2	2.13	0.48
1:E:211:PRO:HG2	1:E:212:ALA:H	1.79	0.48
1:E:50:SER:O	1:E:51:GLU:HG2	2.14	0.48
1:H:15:LEU:C	1:H:15:LEU:HD23	2.34	0.48
1:K:128:HIS:ND1	1:L:76:ILE:HG22	2.29	0.47
1:I:24:ARG:O	1:I:28:LEU:HG	2.14	0.47
1:B:59:PHE:C	1:B:61:LYS:H	2.17	0.47
1:A:193:LEU:HD11	1:A:222:ILE:HD13	1.96	0.47
1:H:104:ASP:OD1	1:H:104:ASP:N	2.40	0.47
1:E:14:ARG:HH21	1:E:193:LEU:HB3	1.79	0.47
1:H:23:ASN:OD1	1:H:26:ASP:HB2	2.14	0.47
1:G:34:VAL:C	1:G:36:GLU:H	2.17	0.47
1:G:180:PRO:HA	1:G:200:ILE:HB	1.96	0.47
1:H:12:MET:O	1:H:13:ASN:HB2	2.13	0.47
1:B:191:GLU:HG2	1:B:194:ARG:NH1	2.29	0.47
1:B:88:PHE:O	1:B:91:GLY:N	2.40	0.47
1:K:45:TYR:N	1:K:46:PRO:CD	2.76	0.47
1:F:29:ARG:O	1:F:33:GLU:HG3	2.14	0.47
1:E:128:HIS:HB2	1:E:129:PRO:CD	2.34	0.47
1:E:171:ILE:C	1:E:171:ILE:HD12	2.35	0.47
1:H:24:ARG:HG3	1:H:51:GLU:CD	2.35	0.47
1:G:34:VAL:CG1	1:G:212:ALA:HA	2.41	0.47
1:E:23:ASN:HD21	1:E:26:ASP:H	1.61	0.47
1:B:155:VAL:HG22	1:B:178:ILE:CG1	2.44	0.47
1:D:45:TYR:N	1:D:46:PRO:CD	2.77	0.47
1:F:216:ALA:C	1:F:219:ILE:HG22	2.34	0.47
1:D:13:ASN:OD1	1:D:219:ILE:HD13	2.14	0.47
1:K:151:VAL:HB	1:K:154:TYR:OH	2.14	0.47
1:I:160:ARG:HE	1:I:163:ARG:CG	2.22	0.47
1:M:215:ALA:O	1:M:219:ILE:HG13	2.15	0.47
1:L:36:GLU:HB2	1:L:37:TYR:CD1	2.50	0.47
1:D:201:VAL:HG11	1:D:205:ILE:HG13	1.96	0.47
1:K:81:GLU:HG3	1:K:112:VAL:HG22	1.97	0.47
1:B:24:ARG:O	1:B:27:ALA:HB3	2.15	0.47
1:B:216:ALA:O	1:B:220:GLU:HG2	2.15	0.47
1:J:220:GLU:OE2	1:J:223:LYS:HG3	2.15	0.47
1:M:72:LYS:HB3	1:M:98:HIS:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:GLY:H	1:J:104:ASP:CG	2.17	0.47
1:C:191:GLU:OE2	1:C:194:ARG:NH1	2.47	0.47
1:E:222:ILE:CG2	1:E:225:LEU:HD13	2.45	0.47
1:J:193:LEU:HD11	1:J:222:ILE:CD1	2.45	0.47
1:I:132:GLU:HG2	1:I:133:MET:N	2.29	0.47
1:C:37:TYR:CE2	1:C:216:ALA:HB2	2.49	0.47
1:C:18:ALA:HB3	1:C:202:GLY:CA	2.44	0.47
1:B:180:PRO:HG3	2:B:229:2OM:O71	2.15	0.47
1:G:162:GLU:HG2	1:G:163:ARG:N	2.30	0.47
1:I:78:GLU:HG2	1:J:203:ARG:NH1	2.30	0.47
1:H:176:PHE:HA	1:H:197:ASP:OD2	2.15	0.47
1:H:182:VAL:CG1	1:H:189:PRO:HG3	2.45	0.47
1:L:162:GLU:N	1:L:162:GLU:CD	2.69	0.47
1:C:19:MET:HA	1:C:19:MET:CE	2.45	0.47
1:K:21:LEU:O	1:K:47:LEU:HD13	2.15	0.46
1:H:12:MET:H	1:H:39:ASP:CG	2.18	0.46
1:D:206:TYR:CD1	1:D:207:LEU:HG	2.51	0.46
1:L:141:GLU:HA	1:L:144:ARG:NH2	2.30	0.46
1:K:97:VAL:HG12	1:K:98:HIS:O	2.16	0.46
1:I:134:PHE:CD2	1:J:138:ALA:HB1	2.51	0.46
1:D:21:LEU:O	1:D:47:LEU:HD13	2.14	0.46
1:I:39:ASP:HB2	1:I:66:ARG:HH21	1.80	0.46
1:G:81:GLU:HG2	1:G:112:VAL:CG2	2.45	0.46
1:J:217:GLY:O	1:J:220:GLU:HB2	2.15	0.46
1:K:80:ASN:ND2	1:K:105:SER:HB3	2.31	0.46
1:C:21:LEU:HG	1:C:206:TYR:CD1	2.51	0.46
1:H:152:LYS:HB3	1:H:152:LYS:NZ	2.30	0.46
1:K:222:ILE:HG13	1:K:222:ILE:O	2.16	0.46
1:F:124:THR:OG1	1:F:167:LEU:HD13	2.16	0.46
1:L:183:GLY:O	1:L:204:SER:N	2.48	0.46
1:G:110:LEU:CD2	1:G:120:VAL:HG21	2.43	0.46
1:K:166:ARG:NH1	1:K:166:ARG:HG3	2.31	0.46
1:J:189:PRO:O	1:J:193:LEU:HG	2.16	0.46
1:G:34:VAL:HG23	1:G:38:ILE:HD11	1.97	0.46
1:B:87:THR:HG21	1:B:95:ILE:HD12	1.98	0.46
1:L:128:HIS:CE1	1:L:131:ALA:HB2	2.51	0.46
1:F:166:ARG:O	1:F:170:ILE:HG13	2.15	0.46
1:F:37:TYR:CE2	1:F:216:ALA:HA	2.51	0.46
1:E:118:ARG:NH2	1:G:118:ARG:NE	2.63	0.46
1:L:189:PRO:O	1:L:193:LEU:HG	2.16	0.46
1:G:206:TYR:CD1	1:G:207:LEU:HG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ILE:HG22	1:B:206:TYR:N	2.31	0.46
1:I:100:PHE:N	1:I:101:PRO:CD	2.79	0.46
1:D:62:ARG:HH11	1:D:62:ARG:HG2	1.81	0.46
1:I:205:ILE:HD13	1:I:214:ALA:HB1	1.97	0.46
1:A:224:ASP:N	1:A:224:ASP:OD2	2.49	0.46
1:F:188:ASP:C	1:F:190:GLY:H	2.19	0.46
1:A:72:LYS:HB3	1:A:98:HIS:CD2	2.50	0.46
1:M:88:PHE:CD1	1:M:118:ARG:HG3	2.51	0.46
1:G:49:LEU:O	1:H:53:MET:HG3	2.16	0.46
1:B:13:ASN:HD22	1:B:219:ILE:CG1	2.29	0.46
1:C:81:GLU:HG3	1:C:108:ALA:HB1	1.98	0.46
1:G:182:VAL:HG21	1:G:199:ILE:HB	1.98	0.46
1:D:222:ILE:HA	1:D:225:LEU:HD13	1.98	0.46
1:D:181:GLY:O	1:D:185:GLN:HB2	2.15	0.46
1:L:168:ARG:HD2	1:L:195:PHE:O	2.16	0.46
1:F:125:GLU:O	1:F:157:PRO:HD3	2.15	0.46
1:I:158:SER:OG	1:I:181:GLY:HA2	2.15	0.46
1:E:136:GLN:HA	1:E:136:GLN:NE2	2.31	0.46
1:G:37:TYR:CE2	1:G:216:ALA:HB2	2.51	0.46
1:B:81:GLU:HG2	1:B:108:ALA:HB1	1.98	0.46
1:J:140:ASP:OD2	1:J:170:ILE:HD11	2.16	0.46
1:K:163:ARG:HB3	1:K:163:ARG:NH1	2.30	0.45
1:D:24:ARG:NH1	1:D:24:ARG:HG2	2.32	0.45
1:A:24:ARG:NH1	1:A:24:ARG:HG2	2.31	0.45
1:B:214:ALA:C	1:B:216:ALA:H	2.19	0.45
1:H:78:GLU:H	1:H:78:GLU:CD	2.20	0.45
1:F:16:ILE:HG23	1:F:40:THR:HG22	1.97	0.45
1:K:120:VAL:O	1:K:120:VAL:HG12	2.15	0.45
1:E:102:GLY:O	1:E:106:VAL:HG23	2.16	0.45
1:H:61:LYS:HZ1	1:L:10:ASP:N	2.13	0.45
1:D:182:VAL:CG1	1:D:189:PRO:HG3	2.46	0.45
1:D:144:ARG:NH2	1:D:166:ARG:NH2	2.64	0.45
1:F:85:ARG:O	1:F:89:LYS:HB2	2.15	0.45
1:B:206:TYR:CE1	1:B:207:LEU:HG	2.51	0.45
1:G:166:ARG:HD2	1:G:166:ARG:HA	1.86	0.45
1:E:42:LYS:HG2	1:E:70:ASP:HB2	1.97	0.45
1:E:55:ILE:HG13	1:E:55:ILE:O	2.17	0.45
1:A:210:ASN:ND2	1:A:213:ALA:HB2	2.32	0.45
1:H:203:ARG:O	1:H:207:LEU:HB2	2.17	0.45
1:G:23:ASN:HD21	1:G:26:ASP:CB	2.27	0.45
1:D:129:PRO:O	1:D:131:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ARG:HA	1:D:206:TYR:CE1	2.51	0.45
1:E:72:LYS:HE2	1:F:75:ASP:CG	2.37	0.45
1:K:125:GLU:HA	1:K:135:ILE:HG22	1.97	0.45
1:F:88:PHE:O	1:F:91:GLY:N	2.32	0.45
1:F:78:GLU:H	1:F:78:GLU:CD	2.19	0.45
1:F:168:ARG:HA	1:F:171:ILE:HG12	1.99	0.45
1:F:12:MET:HG2	1:F:37:TYR:O	2.16	0.45
1:G:29:ARG:NH1	1:G:33:GLU:OE2	2.49	0.45
1:J:214:ALA:C	1:J:216:ALA:H	2.18	0.45
1:G:156:GLY:O	1:G:179:SER:HB2	2.16	0.45
1:F:55:ILE:HD11	1:F:59:PHE:HE1	1.81	0.45
1:B:208:ALA:O	1:B:210:ASN:N	2.50	0.45
1:E:98:HIS:CE1	1:E:123:LEU:HD23	2.52	0.45
1:H:102:GLY:O	1:H:106:VAL:HG23	2.15	0.45
1:D:167:LEU:CD1	1:D:171:ILE:HD13	2.47	0.45
1:L:100:PHE:N	1:L:101:PRO:CD	2.80	0.45
1:K:99:GLY:C	1:K:101:PRO:HD2	2.37	0.45
1:C:220:GLU:OE2	1:C:223:LYS:HD2	2.15	0.45
1:B:88:PHE:HB3	1:B:116:MET:HE2	1.98	0.45
1:C:21:LEU:HA	1:C:21:LEU:HD23	1.84	0.45
1:H:78:GLU:O	1:H:82:LYS:HG3	2.17	0.45
1:I:215:ALA:O	1:I:219:ILE:HG22	2.17	0.45
1:F:122:LEU:HB2	1:F:151:VAL:HG11	1.98	0.45
1:J:163:ARG:NH1	1:J:163:ARG:HB3	2.32	0.45
1:L:177:LEU:HD12	1:L:196:ALA:HA	1.97	0.45
1:J:23:ASN:OD1	1:J:26:ASP:HB2	2.17	0.45
1:F:159:THR:HG22	1:F:159:THR:O	2.17	0.45
1:J:164:LEU:HD21	1:J:192:THR:HG23	1.99	0.45
1:K:130:GLY:C	1:K:132:GLU:H	2.20	0.45
1:K:122:LEU:HD12	1:K:123:LEU:H	1.82	0.44
1:G:180:PRO:CA	1:G:200:ILE:HB	2.46	0.44
1:L:99:GLY:HA3	1:L:142:ILE:HG21	1.99	0.44
1:L:140:ASP:O	1:L:144:ARG:NH1	2.50	0.44
1:I:193:LEU:CD1	1:I:222:ILE:HD13	2.47	0.44
1:E:97:VAL:HG12	1:E:98:HIS:N	2.32	0.44
1:H:155:VAL:HG22	1:H:178:ILE:HD11	1.99	0.44
1:G:155:VAL:HA	1:G:178:ILE:O	2.17	0.44
1:F:45:TYR:HA	1:F:48:VAL:HG22	1.98	0.44
1:F:201:VAL:CG1	1:F:204:SER:HB2	2.47	0.44
1:J:224:ASP:O	1:J:225:LEU:HD23	2.18	0.44
1:J:72:LYS:NZ	2:J:229:2OM:H6	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:LEU:HD12	1:D:177:LEU:HD22	1.99	0.44
1:L:184:ALA:HB2	1:L:203:ARG:HB2	1.99	0.44
1:F:19:MET:CE	1:F:30:VAL:HB	2.47	0.44
1:K:24:ARG:CB	1:K:24:ARG:NH1	2.80	0.44
1:D:24:ARG:HH11	1:D:24:ARG:HG2	1.83	0.44
1:G:100:PHE:N	1:G:101:PRO:CD	2.80	0.44
1:E:218:ILE:O	1:E:221:SER:HB2	2.17	0.44
1:H:48:VAL:HG11	1:H:53:MET:SD	2.58	0.44
1:B:89:LYS:C	1:B:91:GLY:H	2.20	0.44
1:J:193:LEU:HD21	1:J:199:ILE:HG23	2.00	0.44
1:F:211:PRO:HA	1:F:214:ALA:HB2	1.97	0.44
1:H:163:ARG:CA	1:H:163:ARG:HH11	2.21	0.44
1:K:113:ALA:HB2	1:K:120:VAL:CG2	2.48	0.44
1:I:177:LEU:N	1:I:197:ASP:OD2	2.37	0.44
1:H:70:ASP:OD1	1:H:72:LYS:NZ	2.49	0.44
1:I:113:ALA:HB2	1:I:120:VAL:HG23	1.99	0.44
1:L:162:GLU:H	1:L:162:GLU:CD	2.20	0.44
1:H:28:LEU:O	1:H:31:THR:HB	2.17	0.44
1:G:95:ILE:HG23	1:G:95:ILE:O	2.17	0.44
1:L:38:ILE:O	1:L:38:ILE:HD12	2.17	0.44
1:I:191:GLU:C	1:I:191:GLU:OE2	2.56	0.44
1:M:107:ARG:HH21	1:M:149:LEU:CD2	2.30	0.44
1:I:118:ARG:HH11	1:I:118:ARG:HG3	1.83	0.44
1:F:201:VAL:HG13	1:F:204:SER:HB2	2.00	0.44
1:I:157:PRO:HB2	1:I:159:THR:HG23	1.99	0.44
1:G:206:TYR:CE1	1:G:207:LEU:HG	2.53	0.44
1:C:78:GLU:CD	1:C:78:GLU:H	2.21	0.44
1:L:29:ARG:NH1	1:L:29:ARG:HB3	2.33	0.44
1:B:57:ALA:O	1:B:61:LYS:HE2	2.18	0.44
1:H:30:VAL:HG13	1:H:211:PRO:HB3	2.00	0.44
1:E:45:TYR:N	1:E:46:PRO:CD	2.80	0.44
1:B:205:ILE:CD1	1:B:215:ALA:HB2	2.46	0.44
1:D:159:THR:HG22	1:D:185:GLN:O	2.17	0.44
1:K:55:ILE:O	1:K:58:GLU:HB3	2.18	0.44
1:L:85:ARG:HH11	1:L:85:ARG:HG2	1.82	0.44
1:E:222:ILE:HG22	1:E:222:ILE:O	2.18	0.44
1:L:220:GLU:C	1:L:222:ILE:H	2.21	0.44
1:D:219:ILE:HG22	1:D:223:LYS:CG	2.48	0.44
1:G:153:ASN:HA	1:G:176:PHE:O	2.18	0.44
1:L:45:TYR:N	1:L:46:PRO:CD	2.81	0.44
1:K:43:ILE:CD1	1:K:67:ILE:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ARG:O	1:C:169:GLU:HB2	2.17	0.44
1:B:225:LEU:HD12	1:B:225:LEU:N	2.32	0.43
1:E:13:ASN:HD22	1:E:219:ILE:HG23	1.83	0.43
1:J:124:THR:HG22	1:J:142:ILE:HG22	1.99	0.43
1:G:156:GLY:O	1:G:179:SER:CB	2.66	0.43
1:F:128:HIS:O	1:F:131:ALA:CB	2.66	0.43
1:L:138:ALA:C	1:L:140:ASP:H	2.22	0.43
1:K:152:LYS:NZ	1:K:175:SER:HA	2.33	0.43
1:I:143:ALA:O	1:I:147:VAL:HG23	2.18	0.43
1:K:126:MET:HE1	1:L:75:ASP:HA	1.99	0.43
1:I:67:ILE:N	1:I:67:ILE:HD12	2.33	0.43
1:L:23:ASN:ND2	1:L:26:ASP:OD2	2.51	0.43
1:K:182:VAL:HG11	1:K:199:ILE:HD12	2.00	0.43
1:I:66:ARG:HA	1:I:93:ASP:OD2	2.18	0.43
1:J:56:ILE:O	1:J:60:ARG:HG3	2.18	0.43
1:J:78:GLU:CD	1:J:78:GLU:H	2.20	0.43
1:J:45:TYR:N	1:J:46:PRO:CD	2.81	0.43
1:L:216:ALA:O	1:L:219:ILE:HB	2.18	0.43
1:H:192:THR:C	1:H:194:ARG:H	2.21	0.43
1:K:97:VAL:HG12	1:K:98:HIS:N	2.32	0.43
1:F:129:PRO:C	1:F:131:ALA:N	2.71	0.43
1:J:203:ARG:HB3	1:J:207:LEU:HD12	1.99	0.43
1:E:130:GLY:HA3	1:F:104:ASP:OD1	2.18	0.43
1:F:167:LEU:HA	1:F:170:ILE:HD12	2.00	0.43
1:L:21:LEU:HD21	1:L:206:TYR:CD1	2.53	0.43
1:A:73:VAL:HG12	1:A:80:ASN:OD1	2.19	0.43
1:E:49:LEU:HD23	1:E:49:LEU:HA	1.87	0.43
1:I:78:GLU:H	1:I:78:GLU:CD	2.22	0.43
1:L:129:PRO:C	1:L:131:ALA:H	2.21	0.43
1:G:78:GLU:CD	1:G:78:GLU:H	2.22	0.43
1:K:78:GLU:H	1:K:78:GLU:CD	2.21	0.43
1:J:223:LYS:C	1:J:225:LEU:H	2.22	0.43
1:K:126:MET:HB2	1:K:131:ALA:HB2	2.01	0.43
1:E:26:ASP:HA	1:E:29:ARG:NH1	2.33	0.43
1:E:26:ASP:O	1:E:30:VAL:HG23	2.18	0.43
1:H:36:GLU:HG3	1:H:37:TYR:CE2	2.54	0.43
1:K:149:LEU:N	1:K:149:LEU:CD2	2.80	0.43
1:M:72:LYS:HZ1	2:M:229:2OM:H6	1.83	0.43
1:G:10:ASP:C	1:G:10:ASP:OD2	2.57	0.43
1:F:219:ILE:O	1:F:219:ILE:HG12	2.19	0.43
1:H:160:ARG:HH11	1:H:160:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:LYS:HB3	1:F:98:HIS:CD2	2.53	0.43
1:E:9:MET:HE3	1:E:66:ARG:HH21	1.83	0.43
1:A:72:LYS:HE2	1:B:75:ASP:CG	2.38	0.43
1:D:62:ARG:HG2	1:D:62:ARG:NH1	2.32	0.43
1:A:78:GLU:HG2	1:B:203:ARG:NH1	2.34	0.43
1:L:181:GLY:HA2	1:L:185:GLN:HG3	2.00	0.43
1:L:95:ILE:O	1:L:95:ILE:HG23	2.19	0.43
1:J:222:ILE:O	1:J:225:LEU:N	2.52	0.43
1:F:70:ASP:OD1	1:F:72:LYS:NZ	2.48	0.43
1:L:183:GLY:HA2	1:L:204:SER:CB	2.49	0.43
1:G:21:LEU:HD21	1:G:206:TYR:HB2	2.01	0.43
1:G:165:SER:HB2	1:G:195:PHE:CZ	2.53	0.43
1:D:78:GLU:CD	1:D:78:GLU:H	2.22	0.43
1:K:53:MET:HG3	1:L:49:LEU:O	2.18	0.43
1:L:177:LEU:O	1:L:177:LEU:HD12	2.17	0.43
1:E:78:GLU:H	1:E:78:GLU:CD	2.22	0.43
1:B:35:ARG:HD2	1:B:35:ARG:O	2.18	0.43
1:L:78:GLU:H	1:L:78:GLU:CD	2.22	0.43
1:L:17:LEU:HD22	1:L:34:VAL:HG21	2.01	0.43
1:F:179:SER:HB2	1:F:199:ILE:HG22	2.00	0.43
1:K:123:LEU:HD12	1:K:155:VAL:HB	2.01	0.43
1:B:89:LYS:C	1:B:91:GLY:N	2.72	0.43
1:F:36:GLU:HG3	1:F:37:TYR:CD1	2.53	0.43
1:M:220:GLU:C	1:M:222:ILE:H	2.23	0.43
1:L:38:ILE:CD1	1:L:38:ILE:C	2.88	0.43
1:G:107:ARG:HA	1:G:110:LEU:HD12	2.00	0.43
1:I:189:PRO:C	1:I:191:GLU:H	2.22	0.43
1:A:78:GLU:CD	1:A:78:GLU:H	2.22	0.43
1:B:73:VAL:HG12	1:B:80:ASN:OD1	2.19	0.43
1:L:178:ILE:HG22	1:L:198:ALA:HB3	2.00	0.43
1:K:69:ALA:N	1:K:94:ALA:O	2.46	0.43
1:F:206:TYR:CD1	1:F:206:TYR:C	2.92	0.42
1:L:100:PHE:CG	1:L:101:PRO:HD3	2.54	0.42
1:G:210:ASN:HD22	1:G:213:ALA:CB	2.31	0.42
1:L:138:ALA:C	1:L:140:ASP:N	2.72	0.42
1:E:152:LYS:NZ	1:E:152:LYS:HB2	2.34	0.42
1:B:72:LYS:NZ	2:B:229:2OM:H6	2.34	0.42
1:L:42:LYS:HD3	1:L:200:ILE:HG21	2.02	0.42
1:E:43:ILE:CG2	1:E:48:VAL:HG23	2.49	0.42
1:F:94:ALA:HB2	1:F:119:GLU:HB2	2.01	0.42
1:B:78:GLU:H	1:B:78:GLU:CD	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:GLU:OE2	1:J:220:GLU:HA	2.19	0.42
1:H:132:GLU:HG3	1:H:160:ARG:HH21	1.84	0.42
1:F:180:PRO:HG3	2:F:229:2OM:O71	2.19	0.42
1:K:160:ARG:HB3	1:K:162:GLU:OE1	2.19	0.42
1:J:33:GLU:HB3	1:J:212:ALA:HB2	2.01	0.42
1:G:156:GLY:O	1:G:180:PRO:HD2	2.19	0.42
1:E:17:LEU:HD22	1:E:34:VAL:HG21	2.01	0.42
1:B:61:LYS:C	1:B:63:PHE:H	2.22	0.42
1:A:180:PRO:HG3	2:A:229:2OM:O71	2.19	0.42
1:L:138:ALA:O	1:L:141:GLU:N	2.52	0.42
1:B:208:ALA:C	1:B:210:ASN:N	2.71	0.42
1:B:89:LYS:O	1:D:117:GLY:HA3	2.19	0.42
1:K:220:GLU:OE1	1:K:220:GLU:HA	2.18	0.42
1:H:62:ARG:HD2	1:H:63:PHE:CE1	2.54	0.42
1:J:24:ARG:HG2	1:J:55:ILE:HD13	2.02	0.42
1:K:132:GLU:HG2	1:K:160:ARG:NH1	2.34	0.42
1:B:60:ARG:HH22	1:D:60:ARG:HH22	1.67	0.42
1:G:72:LYS:HE2	1:H:75:ASP:CG	2.40	0.42
1:H:37:TYR:HB3	1:H:219:ILE:CD1	2.44	0.42
1:K:125:GLU:HB3	1:K:157:PRO:HG3	2.02	0.42
1:I:166:ARG:O	1:I:169:GLU:HB3	2.19	0.42
1:J:221:SER:O	1:J:222:ILE:HG13	2.20	0.42
1:D:70:ASP:OD1	1:D:72:LYS:NZ	2.51	0.42
1:F:31:THR:HG1	1:F:59:PHE:HE2	1.66	0.42
1:H:72:LYS:HB3	1:H:98:HIS:CD2	2.55	0.42
1:K:125:GLU:O	1:K:157:PRO:HD3	2.20	0.42
1:A:72:LYS:NZ	1:B:75:ASP:OD2	2.52	0.42
1:E:57:ALA:HA	1:E:60:ARG:HD3	2.02	0.42
1:I:45:TYR:N	1:I:46:PRO:CD	2.82	0.42
1:F:29:ARG:HG2	1:F:33:GLU:OE2	2.20	0.42
1:J:174:ASP:N	1:J:174:ASP:OD1	2.37	0.42
1:G:66:ARG:HA	1:G:93:ASP:OD2	2.19	0.42
1:L:164:LEU:HD23	1:L:195:PHE:CD1	2.54	0.42
1:E:221:SER:C	1:E:222:ILE:HG13	2.39	0.42
1:E:193:LEU:HD12	1:E:222:ILE:HG21	2.02	0.42
1:E:222:ILE:HG22	1:E:225:LEU:HB2	2.02	0.42
1:F:193:LEU:HA	1:F:196:ALA:HB3	2.01	0.42
1:F:216:ALA:O	1:F:219:ILE:HG22	2.20	0.42
1:M:180:PRO:HG3	2:M:229:2OM:O71	2.20	0.42
1:G:85:ARG:O	1:G:89:LYS:HB2	2.19	0.42
1:H:15:LEU:HD22	1:H:38:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:CG	1:C:108:ALA:HB1	2.50	0.42
1:K:55:ILE:HG23	1:K:56:ILE:N	2.33	0.42
1:D:100:PHE:CG	1:D:101:PRO:HD3	2.55	0.42
1:K:123:LEU:HD21	1:K:126:MET:HG2	2.02	0.42
1:E:13:ASN:HD22	1:E:219:ILE:CG2	2.32	0.42
1:M:72:LYS:O	1:M:73:VAL:C	2.58	0.42
1:I:130:GLY:N	1:J:104:ASP:OD2	2.42	0.42
1:I:88:PHE:HB3	1:I:118:ARG:NH1	2.35	0.42
1:C:123:LEU:HA	1:C:155:VAL:HB	2.02	0.42
1:E:160:ARG:HB3	1:E:163:ARG:HB2	2.01	0.42
1:K:225:LEU:HD12	1:K:225:LEU:N	2.34	0.42
1:L:171:ILE:CD1	1:L:177:LEU:HD23	2.46	0.42
1:F:190:GLY:HA2	1:F:222:ILE:HG21	2.02	0.42
1:M:118:ARG:HH11	1:M:118:ARG:HD3	1.77	0.42
1:I:121:PHE:HB3	1:I:155:VAL:HG23	2.01	0.42
1:J:20:ASP:HB2	1:J:206:TYR:OH	2.19	0.42
1:F:133:MET:HB3	1:F:134:PHE:CE1	2.55	0.42
1:E:193:LEU:HD12	1:E:222:ILE:HD13	2.01	0.42
1:D:167:LEU:HD12	1:D:177:LEU:CD2	2.50	0.42
1:G:189:PRO:HG2	1:G:218:ILE:CD1	2.47	0.42
1:G:72:LYS:HB3	1:G:98:HIS:CD2	2.54	0.42
1:E:100:PHE:HB3	1:E:101:PRO:HD3	2.02	0.42
1:F:23:ASN:HD21	1:F:26:ASP:HB2	1.85	0.42
1:K:211:PRO:O	1:K:214:ALA:HB3	2.20	0.42
1:F:40:THR:OG1	1:F:66:ARG:HG3	2.20	0.42
1:J:193:LEU:CD2	1:J:199:ILE:HG23	2.50	0.42
1:H:164:LEU:HD23	1:H:195:PHE:CD1	2.39	0.42
1:H:192:THR:HG21	1:H:199:ILE:HG22	2.00	0.42
1:K:180:PRO:HA	1:K:200:ILE:HB	2.02	0.42
1:F:128:HIS:O	1:F:131:ALA:HB3	2.20	0.42
1:B:30:VAL:O	1:B:34:VAL:HG22	2.20	0.42
1:G:210:ASN:HD22	1:G:213:ALA:H	1.67	0.42
1:G:22:MET:CE	1:H:82:LYS:HB3	2.49	0.42
1:M:45:TYR:N	1:M:46:PRO:CD	2.82	0.42
1:C:45:TYR:N	1:C:46:PRO:CD	2.83	0.42
1:L:89:LYS:HG2	1:L:89:LYS:O	2.20	0.42
1:J:163:ARG:CB	1:J:163:ARG:NH1	2.83	0.41
1:F:158:SER:C	1:F:160:ARG:H	2.23	0.41
1:C:118:ARG:NH2	1:F:118:ARG:NH1	2.67	0.41
1:K:79:THR:O	1:K:83:ILE:HG13	2.19	0.41
1:C:188:ASP:HA	1:C:189:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:78:GLU:H	1:M:78:GLU:CD	2.22	0.41
1:F:72:LYS:NZ	2:F:229:2OM:H6	2.33	0.41
1:K:163:ARG:HH11	1:K:163:ARG:CA	2.32	0.41
1:I:133:MET:HB3	1:I:134:PHE:CE1	2.54	0.41
1:M:10:ASP:C	1:M:10:ASP:OD2	2.57	0.41
1:B:24:ARG:HB2	1:B:51:GLU:CD	2.41	0.41
1:E:45:TYR:O	1:E:46:PRO:C	2.56	0.41
1:D:125:GLU:OE2	1:D:160:ARG:NH1	2.49	0.41
1:I:49:LEU:HB3	1:J:53:MET:HE2	2.02	0.41
1:B:94:ALA:HA	1:B:119:GLU:O	2.20	0.41
1:D:155:VAL:HG13	1:D:180:PRO:HD3	2.02	0.41
1:K:29:ARG:HH11	1:K:29:ARG:HB3	1.86	0.41
1:D:220:GLU:HA	1:D:223:LYS:CD	2.48	0.41
1:K:37:TYR:HB3	1:K:219:ILE:HD11	2.01	0.41
1:D:153:ASN:OD1	1:D:176:PHE:HB3	2.21	0.41
1:K:203:ARG:HG3	1:K:206:TYR:OH	2.20	0.41
1:L:84:CYS:HG	1:L:109:CYS:HG	1.65	0.41
1:M:214:ALA:O	1:M:218:ILE:HG13	2.20	0.41
1:E:182:VAL:CG1	1:E:189:PRO:HD3	2.50	0.41
1:E:193:LEU:CD2	1:E:199:ILE:HG23	2.50	0.41
1:F:184:ALA:HB2	1:F:203:ARG:HB2	2.03	0.41
1:F:162:GLU:CG	1:F:163:ARG:N	2.81	0.41
1:K:112:VAL:HG12	1:K:116:MET:HE3	2.01	0.41
1:D:163:ARG:CA	1:D:163:ARG:HH11	2.33	0.41
1:D:188:ASP:HA	1:D:189:PRO:HD3	1.90	0.41
1:J:24:ARG:HB3	1:J:24:ARG:CZ	2.49	0.41
1:J:88:PHE:O	1:J:89:LYS:C	2.58	0.41
1:A:45:TYR:N	1:A:46:PRO:CD	2.84	0.41
1:K:84:CYS:HB3	1:K:88:PHE:CE2	2.56	0.41
1:M:100:PHE:HB3	1:M:101:PRO:HD3	2.01	0.41
1:K:222:ILE:HD12	1:K:225:LEU:HD13	2.02	0.41
1:C:210:ASN:HB3	1:C:213:ALA:CB	2.49	0.41
1:F:15:LEU:HA	1:F:199:ILE:O	2.21	0.41
1:I:159:THR:HG22	1:I:185:GLN:HB3	2.03	0.41
1:I:203:ARG:O	1:I:207:LEU:HB2	2.20	0.41
1:L:225:LEU:HD23	1:L:225:LEU:N	2.35	0.41
1:H:35:ARG:HH12	1:H:39:ASP:HA	1.85	0.41
1:L:30:VAL:HG11	1:L:206:TYR:HA	2.01	0.41
1:I:78:GLU:HG2	1:J:203:ARG:HH12	1.86	0.41
1:F:164:LEU:HD11	1:F:179:SER:OG	2.20	0.41
1:I:158:SER:OG	1:I:180:PRO:O	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:LYS:HE2	1:D:75:ASP:CG	2.41	0.41
1:B:161:PRO:HB3	1:B:191:GLU:CD	2.40	0.41
1:I:129:PRO:O	1:I:131:ALA:N	2.52	0.41
1:H:43:ILE:CG2	1:H:48:VAL:HG23	2.51	0.41
1:D:182:VAL:HG13	1:D:187:GLY:O	2.20	0.41
1:J:125:GLU:O	1:J:157:PRO:HD3	2.20	0.41
1:G:181:GLY:HA2	1:G:185:GLN:NE2	2.35	0.41
1:B:163:ARG:NH1	1:B:163:ARG:HB3	2.35	0.41
1:L:35:ARG:NH1	1:L:38:ILE:O	2.53	0.41
1:M:11:VAL:HG21	1:M:16:ILE:HD11	2.02	0.41
1:K:203:ARG:HG3	1:K:206:TYR:CZ	2.55	0.41
1:L:188:ASP:OD2	1:L:191:GLU:HB2	2.21	0.41
1:M:125:GLU:HB3	1:M:157:PRO:HD3	2.03	0.41
1:J:124:THR:OG1	1:J:167:LEU:HD11	2.20	0.41
1:B:72:LYS:HB3	1:B:98:HIS:CD2	2.54	0.41
1:D:13:ASN:O	1:D:14:ARG:C	2.59	0.41
1:K:104:ASP:OD1	1:K:104:ASP:N	2.50	0.41
1:L:70:ASP:OD1	1:L:72:LYS:NZ	2.54	0.41
1:J:49:LEU:HD23	1:J:49:LEU:HA	1.83	0.41
1:I:136:GLN:O	1:I:136:GLN:OE1	2.38	0.41
1:K:169:GLU:HG3	1:K:170:ILE:N	2.36	0.41
1:K:193:LEU:HA	1:K:193:LEU:HD23	1.87	0.41
1:J:160:ARG:HB3	1:J:163:ARG:HG2	2.03	0.41
1:J:193:LEU:HD11	1:J:222:ILE:HD13	2.03	0.41
1:F:205:ILE:HA	1:F:214:ALA:HB1	2.03	0.41
1:E:26:ASP:HA	1:E:29:ARG:HH12	1.86	0.41
1:K:107:ARG:NH2	1:K:149:LEU:O	2.53	0.41
1:E:100:PHE:CE2	1:F:100:PHE:HB2	2.56	0.41
1:I:201:VAL:HG11	1:I:218:ILE:HD13	2.02	0.41
1:H:29:ARG:HG2	1:H:33:GLU:OE2	2.21	0.41
1:F:51:GLU:HA	1:F:51:GLU:OE1	2.20	0.41
1:A:121:PHE:CD2	1:A:153:ASN:HB3	2.55	0.41
1:A:34:VAL:HG23	1:A:38:ILE:HD12	2.03	0.41
1:G:55:ILE:HD11	1:G:59:PHE:HE1	1.86	0.41
1:J:152:LYS:HB3	1:J:152:LYS:HE2	1.86	0.41
1:J:159:THR:O	1:J:160:ARG:HG3	2.21	0.41
1:B:163:ARG:CA	1:B:163:ARG:HH11	2.28	0.41
1:F:211:PRO:C	1:F:213:ALA:H	2.24	0.41
1:D:216:ALA:O	1:D:220:GLU:HB2	2.21	0.41
1:B:61:LYS:C	1:B:63:PHE:N	2.74	0.41
1:E:142:ILE:O	1:E:145:MET:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:73:VAL:HG12	1:M:80:ASN:OD1	2.20	0.41
1:K:66:ARG:HG3	1:K:66:ARG:NH1	2.36	0.41
1:E:49:LEU:O	1:F:53:MET:HG3	2.21	0.41
1:G:53:MET:C	1:G:55:ILE:N	2.74	0.41
1:D:73:VAL:HG12	1:D:80:ASN:OD1	2.21	0.41
1:L:159:THR:C	1:L:161:PRO:HD3	2.41	0.41
1:E:104:ASP:N	1:E:104:ASP:OD1	2.54	0.40
1:I:141:GLU:HB3	1:J:134:PHE:CE2	2.50	0.40
1:I:128:HIS:HB3	1:J:76:ILE:HG22	2.03	0.40
1:D:222:ILE:C	1:D:224:ASP:N	2.73	0.40
1:L:49:LEU:HD23	1:L:49:LEU:HA	1.87	0.40
1:E:35:ARG:NH1	1:E:38:ILE:O	2.55	0.40
1:A:167:LEU:O	1:A:171:ILE:HG12	2.22	0.40
1:D:18:ALA:HB3	1:D:202:GLY:CA	2.51	0.40
1:F:164:LEU:HD23	1:F:195:PHE:CE1	2.54	0.40
1:K:70:ASP:OD1	1:K:72:LYS:NZ	2.53	0.40
1:K:81:GLU:HG3	1:K:112:VAL:CG2	2.51	0.40
1:K:217:GLY:O	1:K:220:GLU:N	2.54	0.40
1:H:32:GLY:HA2	1:H:63:PHE:HE2	1.86	0.40
1:I:160:ARG:O	1:I:163:ARG:HB2	2.21	0.40
1:E:13:ASN:ND2	1:E:219:ILE:CG2	2.84	0.40
1:L:203:ARG:O	1:L:205:ILE:N	2.54	0.40
1:D:163:ARG:CB	1:D:163:ARG:NH1	2.83	0.40
1:E:72:LYS:NZ	2:E:229:2OM:H6	2.35	0.40
1:I:100:PHE:HB2	1:J:100:PHE:CZ	2.56	0.40
1:E:49:LEU:HD22	1:F:53:MET:HE2	2.03	0.40
1:J:166:ARG:O	1:J:170:ILE:HG13	2.21	0.40
1:M:23:ASN:ND2	1:M:26:ASP:OD2	2.41	0.40
1:G:144:ARG:HH11	1:G:144:ARG:HG2	1.85	0.40
1:J:183:GLY:HA3	1:J:204:SER:OG	2.21	0.40
1:M:224:ASP:C	1:M:225:LEU:HD12	2.41	0.40
1:K:193:LEU:HD12	1:K:222:ILE:CG1	2.26	0.40
1:J:163:ARG:CA	1:J:163:ARG:NH1	2.75	0.40
1:J:72:LYS:HB3	1:J:98:HIS:CD2	2.56	0.40
1:L:37:TYR:HB3	1:L:219:ILE:CD1	2.47	0.40
1:I:188:ASP:CB	1:I:189:PRO:HD2	2.49	0.40
1:C:24:ARG:HB2	1:C:51:GLU:CD	2.42	0.40
1:J:104:ASP:OD1	1:J:104:ASP:N	2.54	0.40
1:F:88:PHE:CD1	1:F:118:ARG:HG3	2.56	0.40
1:K:201:VAL:CG1	1:K:204:SER:HB2	2.52	0.40
1:M:21:LEU:HD23	1:M:21:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:191:GLU:O	1:J:194:ARG:HB3	2.21	0.40
1:G:100:PHE:HB3	1:H:100:PHE:CE2	2.57	0.40
1:F:49:LEU:HD23	1:F:49:LEU:HA	1.91	0.40
1:G:18:ALA:HA	1:G:42:LYS:HB3	2.02	0.40
1:H:182:VAL:HG11	1:H:189:PRO:HG3	2.02	0.40
1:E:181:GLY:HA2	1:E:185:GLN:HB2	2.04	0.40
1:A:211:PRO:O	1:A:214:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/228 (96%)	209 (96%)	9 (4%)	0	100	100
1	B	214/228 (94%)	181 (85%)	27 (13%)	6 (3%)	6	9
1	C	216/228 (95%)	196 (91%)	18 (8%)	2 (1%)	21	37
1	D	213/228 (93%)	186 (87%)	21 (10%)	6 (3%)	6	9
1	E	215/228 (94%)	193 (90%)	18 (8%)	4 (2%)	10	16
1	F	215/228 (94%)	178 (83%)	28 (13%)	9 (4%)	3	4
1	G	215/228 (94%)	193 (90%)	18 (8%)	4 (2%)	10	16
1	H	214/228 (94%)	179 (84%)	32 (15%)	3 (1%)	14	24
1	I	210/228 (92%)	187 (89%)	19 (9%)	4 (2%)	10	16
1	J	216/228 (95%)	186 (86%)	26 (12%)	4 (2%)	10	16
1	K	214/228 (94%)	182 (85%)	28 (13%)	4 (2%)	10	16
1	L	214/228 (94%)	174 (81%)	31 (14%)	9 (4%)	3	4
1	M	215/228 (94%)	205 (95%)	10 (5%)	0	100	100
All	All	2789/2964 (94%)	2449 (88%)	285 (10%)	55 (2%)	9	15



All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	224	ASP
1	F	14	ARG
1	I	129	PRO
1	I	184	ALA
1	L	180	PRO
1	L	181	GLY
1	L	184	ALA
1	L	189	PRO
1	B	34	VAL
1	D	189	PRO
1	F	19	MET
1	F	222	ILE
1	K	130	GLY
1	K	138	ALA
1	B	60	ARG
1	B	206	TYR
1	D	203	ARG
1	D	211	PRO
1	F	159	THR
1	G	46	PRO
1	G	211	PRO
1	I	193	LEU
1	J	222	ILE
1	L	182	VAL
1	L	185	GLN
1	L	204	SER
1	B	209	ASP
1	C	9	MET
1	D	130	GLY
1	F	25	ASP
1	G	115	GLU
1	I	130	GLY
1	L	36	GLU
1	E	189	PRO
1	E	223	LYS
1	F	60	ARG
1	H	222	ILE
1	J	14	ARG
1	B	64	GLY
1	D	190	GLY
1	F	205	ILE
1	J	139	ALA

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Mol	Chain	Res	Type
1	J	189	PRO
1	K	120	VAL
1	L	168	ARG
1	C	189	PRO
1	F	189	PRO
1	B	222	ILE
1	E	211	PRO
1	F	190	GLY
1	D	187	GLY
1	H	135	ILE
1	H	100	PHE
1	G	56	ILE
1	K	101	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/182 (96%)	167 (96%)	7 (4%)	38	64
1	B	170/182 (93%)	163 (96%)	7 (4%)	37	63
1	C	172/182 (94%)	165 (96%)	7 (4%)	37	63
1	D	169/182 (93%)	164 (97%)	5 (3%)	48	76
1	E	171/182 (94%)	165 (96%)	6 (4%)	43	70
1	F	171/182 (94%)	163 (95%)	8 (5%)	32	56
1	G	171/182 (94%)	166 (97%)	5 (3%)	50	77
1	H	170/182 (93%)	169 (99%)	1 (1%)	90	97
1	I	166/182 (91%)	159 (96%)	7 (4%)	36	62
1	J	172/182 (94%)	168 (98%)	4 (2%)	58	83
1	K	170/182 (93%)	166 (98%)	4 (2%)	57	82
1	L	170/182 (93%)	164 (96%)	6 (4%)	43	70
1	M	171/182 (94%)	169 (99%)	2 (1%)	78	93
All	All	2217/2366 (94%)	2148 (97%)	69 (3%)	47	75

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	29	ARG
1	A	36	GLU
1	A	38	ILE
1	A	81	GLU
1	A	182	VAL
1	A	211	PRO
1	B	19	MET
1	B	29	ARG
1	B	33	GLU
1	B	66	ARG
1	B	85	ARG
1	B	167	LEU
1	B	210	ASN
1	C	19	MET
1	C	62	ARG
1	C	66	ARG
1	C	107	ARG
1	C	167	LEU
1	C	180	PRO
1	C	224	ASP
1	D	37	TYR
1	D	38	ILE
1	D	54	ASP
1	D	58	GLU
1	D	62	ARG
1	E	58	GLU
1	E	81	GLU
1	E	114	GLU
1	E	136	GLN
1	E	209	ASP
1	E	223	LYS
1	F	17	LEU
1	F	38	ILE
1	F	66	ARG
1	F	89	LYS
1	F	193	LEU
1	F	195	PHE
1	F	206	TYR
1	F	210	ASN
1	G	9	MET
1	G	37	TYR

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Mol	Chain	Res	Type
1	G	118	ARG
1	G	220	GLU
1	G	224	ASP
1	H	26	ASP
1	I	81	GLU
1	I	127	SER
1	I	136	GLN
1	I	140	ASP
1	I	141	GLU
1	I	158	SER
1	I	167	LEU
1	J	26	ASP
1	J	66	ARG
1	J	164	LEU
1	J	167	LEU
1	K	24	ARG
1	K	26	ASP
1	K	62	ARG
1	K	148	ASP
1	L	58	GLU
1	L	114	GLU
1	L	162	GLU
1	L	195	PHE
1	L	209	ASP
1	L	223	LYS
1	M	10	ASP
1	M	107	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	136	GLN
1	B	210	ASN
1	C	210	ASN
1	E	13	ASN
1	E	23	ASN
1	E	111	ASN
1	E	136	GLN
1	F	210	ASN
1	G	210	ASN
1	H	210	ASN

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Mol	Chain	Res	Type
1	I	185	GLN
1	J	210	ASN
1	K	136	GLN
1	K	173	GLN
1	L	23	ASN
1	L	98	HIS
1	L	173	GLN
1	M	98	HIS
1	M	210	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	2OM	A	229	-	21,25,25	1.12	2 (9%)	28,38,38	1.78	4 (14%)
2	2OM	B	229	-	21,25,25	1.20	2 (9%)	28,38,38	1.80	4 (14%)
2	2OM	C	229	-	21,25,25	1.11	1 (4%)	28,38,38	1.77	4 (14%)
2	2OM	D	229	-	21,25,25	1.20	4 (19%)	28,38,38	1.82	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2OM	E	229	-	21,25,25	1.12	3 (14%)	28,38,38	1.78	4 (14%)
2	2OM	F	229	-	21,25,25	1.27	4 (19%)	28,38,38	1.84	4 (14%)
2	2OM	G	229	-	21,25,25	1.18	4 (19%)	28,38,38	1.80	4 (14%)
2	2OM	H	229	-	21,25,25	1.15	2 (9%)	28,38,38	1.80	4 (14%)
2	2OM	I	229	-	21,25,25	1.23	3 (14%)	28,38,38	1.80	4 (14%)
2	2OM	J	229	-	21,25,25	1.19	3 (14%)	28,38,38	1.80	4 (14%)
2	2OM	K	229	-	21,25,25	1.23	3 (14%)	28,38,38	1.79	4 (14%)
2	2OM	L	229	-	21,25,25	1.13	2 (9%)	28,38,38	1.82	5 (17%)
2	2OM	M	229	-	21,25,25	1.22	3 (14%)	28,38,38	1.75	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2OM	A	229	-	-	0/10/46/46	0/2/2/2
2	2OM	B	229	-	-	0/10/46/46	0/2/2/2
2	2OM	C	229	-	-	0/10/46/46	0/2/2/2
2	2OM	D	229	-	-	0/10/46/46	0/2/2/2
2	2OM	E	229	-	-	0/10/46/46	0/2/2/2
2	2OM	F	229	-	-	0/10/46/46	0/2/2/2
2	2OM	G	229	-	-	0/10/46/46	0/2/2/2
2	2OM	H	229	-	-	0/10/46/46	0/2/2/2
2	2OM	I	229	-	-	0/10/46/46	0/2/2/2
2	2OM	J	229	-	-	0/10/46/46	0/2/2/2
2	2OM	K	229	-	-	0/10/46/46	0/2/2/2
2	2OM	L	229	-	-	0/10/46/46	0/2/2/2
2	2OM	M	229	-	-	0/10/46/46	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	229	2OM	P-OP3	2.00	1.61	1.54
2	E	229	2OM	C6-N1	2.01	1.50	1.48
2	A	229	2OM	O4'-C1'	2.04	1.47	1.42
2	J	229	2OM	P-OP3	2.05	1.62	1.54
2	G	229	2OM	O4'-C1'	2.05	1.47	1.42
2	H	229	2OM	O4'-C1'	2.05	1.47	1.42
2	B	229	2OM	P-OP3	2.06	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	229	2OM	P-OP3	2.07	1.62	1.54
2	M	229	2OM	P-OP2	2.10	1.62	1.54
2	G	229	2OM	C6-N1	2.14	1.50	1.48
2	L	229	2OM	P-OP2	2.14	1.62	1.54
2	I	229	2OM	P-OP2	2.16	1.62	1.54
2	F	229	2OM	O4'-C1'	2.16	1.47	1.42
2	J	229	2OM	O4'-C1'	2.18	1.47	1.42
2	G	229	2OM	P-OP2	2.19	1.62	1.54
2	D	229	2OM	P-OP2	2.20	1.62	1.54
2	A	229	2OM	C6-N1	2.21	1.50	1.48
2	K	229	2OM	P-OP2	2.22	1.62	1.54
2	E	229	2OM	O4'-C1'	2.22	1.47	1.42
2	F	229	2OM	P-OP2	2.22	1.62	1.54
2	F	229	2OM	C5-C6	2.22	1.56	1.53
2	D	229	2OM	P-OP3	2.23	1.62	1.54
2	D	229	2OM	C6-N1	2.26	1.50	1.48
2	H	229	2OM	C6-N1	2.27	1.50	1.48
2	D	229	2OM	O4'-C1'	2.28	1.47	1.42
2	K	229	2OM	O4'-C1'	2.29	1.47	1.42
2	L	229	2OM	O4'-C1'	2.31	1.47	1.42
2	I	229	2OM	O4'-C1'	2.31	1.47	1.42
2	F	229	2OM	P-OP3	2.32	1.63	1.54
2	B	229	2OM	O4'-C1'	2.36	1.47	1.42
2	J	229	2OM	C6-N1	2.38	1.50	1.48
2	M	229	2OM	O4'-C1'	2.41	1.48	1.42
2	C	229	2OM	C6-N1	2.42	1.50	1.48
2	M	229	2OM	C6-N1	2.47	1.50	1.48
2	I	229	2OM	C6-N1	2.52	1.50	1.48
2	K	229	2OM	C6-N1	2.73	1.50	1.48

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	229	2OM	C4-N3-C2	-4.35	122.20	125.79
2	F	229	2OM	C4-N3-C2	-4.35	122.20	125.79
2	L	229	2OM	C4-N3-C2	-4.29	122.25	125.79
2	G	229	2OM	C4-N3-C2	-4.22	122.31	125.79
2	E	229	2OM	C4-N3-C2	-4.22	122.31	125.79
2	D	229	2OM	C4-N3-C2	-4.22	122.31	125.79
2	K	229	2OM	C4-N3-C2	-4.19	122.33	125.79
2	H	229	2OM	C4-N3-C2	-4.15	122.36	125.79
2	B	229	2OM	C4-N3-C2	-4.14	122.37	125.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	229	2OM	C4-N3-C2	-4.12	122.39	125.79
2	J	229	2OM	C4-N3-C2	-4.08	122.43	125.79
2	M	229	2OM	C4-N3-C2	-3.97	122.52	125.79
2	A	229	2OM	C4-N3-C2	-3.93	122.54	125.79
2	L	229	2OM	O2-C2-N1	-2.03	120.29	123.36
2	B	229	2OM	C5-C6-N1	3.26	113.73	109.15
2	M	229	2OM	C5-C6-N1	3.33	113.83	109.15
2	I	229	2OM	C5-C6-N1	3.34	113.84	109.15
2	C	229	2OM	C5-C6-N1	3.36	113.86	109.15
2	E	229	2OM	C5-C6-N1	3.38	113.90	109.15
2	H	229	2OM	C5-C6-N1	3.39	113.91	109.15
2	G	229	2OM	C5-C6-N1	3.47	114.02	109.15
2	F	229	2OM	C5-C6-N1	3.50	114.07	109.15
2	K	229	2OM	C5-C6-N1	3.51	114.08	109.15
2	A	229	2OM	C5-C6-N1	3.57	114.16	109.15
2	L	229	2OM	C5-C6-N1	3.59	114.20	109.15
2	D	229	2OM	C5-C6-N1	3.60	114.21	109.15
2	J	229	2OM	C5-C6-N1	3.62	114.23	109.15
2	C	229	2OM	C5-C4-N3	3.92	120.77	116.21
2	L	229	2OM	C5-C4-N3	3.94	120.79	116.21
2	A	229	2OM	C5-C4-N3	3.95	120.80	116.21
2	K	229	2OM	C5-C4-N3	3.96	120.81	116.21
2	I	229	2OM	C5-C4-N3	3.97	120.83	116.21
2	G	229	2OM	C5-C4-N3	4.03	120.89	116.21
2	E	229	2OM	C5-C4-N3	4.03	120.89	116.21
2	M	229	2OM	C5-C4-N3	4.04	120.90	116.21
2	H	229	2OM	C5-C4-N3	4.06	120.93	116.21
2	B	229	2OM	C5-C4-N3	4.11	120.99	116.21
2	J	229	2OM	C5-C4-N3	4.12	121.00	116.21
2	F	229	2OM	C5-C4-N3	4.18	121.06	116.21
2	D	229	2OM	C5-C4-N3	4.29	121.20	116.21
2	D	229	2OM	N3-C2-N1	4.69	121.52	116.82
2	E	229	2OM	N3-C2-N1	4.77	121.60	116.82
2	M	229	2OM	N3-C2-N1	4.79	121.62	116.82
2	J	229	2OM	N3-C2-N1	4.80	121.63	116.82
2	G	229	2OM	N3-C2-N1	4.81	121.63	116.82
2	K	229	2OM	N3-C2-N1	4.82	121.65	116.82
2	C	229	2OM	N3-C2-N1	4.87	121.69	116.82
2	A	229	2OM	N3-C2-N1	4.91	121.74	116.82
2	I	229	2OM	N3-C2-N1	4.93	121.75	116.82
2	F	229	2OM	N3-C2-N1	4.96	121.78	116.82
2	L	229	2OM	N3-C2-N1	4.98	121.81	116.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	229	2OM	N3-C2-N1	4.99	121.81	116.82
2	B	229	2OM	N3-C2-N1	4.99	121.82	116.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	229	2OM	2	0
2	B	229	2OM	3	0
2	C	229	2OM	1	0
2	D	229	2OM	2	0
2	E	229	2OM	2	0
2	F	229	2OM	3	0
2	G	229	2OM	2	0
2	H	229	2OM	1	0
2	J	229	2OM	2	0
2	K	229	2OM	2	0
2	L	229	2OM	2	0
2	M	229	2OM	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	220/228 (96%)	-0.18	11 (5%) 32 37	24, 39, 59, 95	0
1	B	216/228 (94%)	0.26	16 (7%) 17 19	25, 50, 83, 110	0
1	C	218/228 (95%)	-0.07	7 (3%) 51 56	30, 45, 71, 94	0
1	D	215/228 (94%)	0.31	18 (8%) 14 14	33, 52, 109, 119	0
1	E	217/228 (95%)	0.31	12 (5%) 29 32	41, 66, 84, 100	0
1	F	217/228 (95%)	0.71	34 (15%) 3 2	39, 67, 111, 113	0
1	G	217/228 (95%)	0.39	14 (6%) 22 25	41, 65, 101, 117	0
1	H	216/228 (94%)	0.27	11 (5%) 32 36	41, 67, 97, 123	0
1	I	212/228 (92%)	0.52	22 (10%) 8 8	31, 66, 113, 139	0
1	J	218/228 (95%)	0.18	12 (5%) 29 32	34, 60, 96, 106	0
1	K	216/228 (94%)	0.38	20 (9%) 11 11	43, 72, 89, 102	0
1	L	216/228 (94%)	0.56	24 (11%) 7 7	42, 80, 110, 128	0
1	M	217/228 (95%)	0.66	23 (10%) 8 8	32, 55, 97, 129	0
All	All	2815/2964 (94%)	0.33	224 (7%) 15 16	24, 61, 101, 139	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	225	LEU	14.4
1	M	224	ASP	9.0
1	I	184	ALA	8.8
1	D	225	LEU	6.8
1	F	34	VAL	6.5
1	F	207	LEU	6.5
1	I	185	GLN	6.4
1	L	193	LEU	6.3
1	M	214	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	L	225	LEU	6.0
1	L	167	LEU	5.8
1	M	207	LEU	5.3
1	D	215	ALA	5.2
1	B	225	LEU	5.2
1	D	207	LEU	4.9
1	K	147	VAL	4.8
1	J	215	ALA	4.8
1	F	208	ALA	4.7
1	I	182	VAL	4.6
1	I	190	GLY	4.6
1	F	217	GLY	4.5
1	F	218	ILE	4.4
1	I	223	LYS	4.4
1	F	37	TYR	4.4
1	G	222	ILE	4.3
1	E	223	LYS	4.3
1	H	224	ASP	4.3
1	I	186	GLY	4.3
1	B	38	ILE	4.3
1	I	181	GLY	4.2
1	B	222	ILE	4.2
1	F	220	GLU	4.2
1	M	9	MET	4.1
1	D	224	ASP	4.1
1	G	209	ASP	4.1
1	G	208	ALA	4.1
1	F	13	ASN	4.1
1	L	195	PHE	4.1
1	D	182	VAL	4.0
1	L	224	ASP	4.0
1	M	37	TYR	4.0
1	E	96	ILE	4.0
1	H	208	ALA	4.0
1	I	222	ILE	3.9
1	F	215	ALA	3.8
1	B	224	ASP	3.8
1	L	21	LEU	3.7
1	F	209	ASP	3.7
1	I	224	ASP	3.7
1	D	214	ALA	3.7
1	K	182	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	14	ARG	3.7
1	F	191	GLU	3.6
1	H	222	ILE	3.6
1	K	224	ASP	3.5
1	M	222	ILE	3.5
1	A	225	LEU	3.5
1	E	189	PRO	3.5
1	L	174	ASP	3.4
1	F	38	ILE	3.4
1	F	222	ILE	3.4
1	K	222	ILE	3.4
1	J	225	LEU	3.3
1	G	218	ILE	3.3
1	K	135	ILE	3.3
1	L	186	GLY	3.3
1	D	181	GLY	3.3
1	H	225	LEU	3.2
1	B	191	GLU	3.2
1	F	22	MET	3.2
1	A	8	VAL	3.2
1	B	217	GLY	3.2
1	G	202	GLY	3.2
1	H	27	ALA	3.2
1	E	216	ALA	3.1
1	F	9	MET	3.1
1	F	159	THR	3.1
1	J	222	ILE	3.1
1	L	142	ILE	3.1
1	I	158	SER	3.1
1	F	206	TYR	3.1
1	E	225	LEU	3.1
1	D	209	ASP	3.1
1	I	210	ASN	3.0
1	D	220	GLU	3.0
1	F	214	ALA	3.0
1	F	36	GLU	3.0
1	M	100	PHE	3.0
1	F	211	PRO	3.0
1	B	74	ALA	3.0
1	H	96	ILE	2.9
1	E	208	ALA	2.9
1	E	222	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	33	GLU	2.9
1	H	209	ASP	2.9
1	L	207	LEU	2.9
1	L	135	ILE	2.9
1	G	28	LEU	2.9
1	D	162	GLU	2.9
1	I	74	ALA	2.9
1	A	73	VAL	2.8
1	K	97	VAL	2.8
1	J	207	LEU	2.8
1	L	161	PRO	2.8
1	M	189	PRO	2.8
1	B	220	GLU	2.8
1	A	69	ALA	2.8
1	G	207	LEU	2.8
1	F	219	ILE	2.7
1	L	190	GLY	2.7
1	M	74	ALA	2.7
1	C	73	VAL	2.7
1	F	29	ARG	2.7
1	J	30	VAL	2.7
1	M	223	LYS	2.7
1	M	73	VAL	2.7
1	M	217	GLY	2.6
1	H	37	TYR	2.6
1	D	11	VAL	2.6
1	J	74	ALA	2.6
1	K	220	GLU	2.6
1	F	15	LEU	2.6
1	E	218	ILE	2.6
1	G	182	VAL	2.6
1	M	209	ASP	2.6
1	C	96	ILE	2.6
1	C	71	PHE	2.6
1	M	97	VAL	2.5
1	H	187	GLY	2.5
1	L	180	PRO	2.5
1	B	215	ALA	2.5
1	J	69	ALA	2.5
1	G	211	PRO	2.5
1	L	164	LEU	2.5
1	I	205	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	223	LYS	2.5
1	I	189	PRO	2.5
1	E	97	VAL	2.5
1	F	162	GLU	2.5
1	B	73	VAL	2.5
1	C	74	ALA	2.5
1	D	189	PRO	2.5
1	D	192	THR	2.5
1	K	152	LYS	2.4
1	I	166	ARG	2.4
1	K	225	LEU	2.4
1	L	97	VAL	2.4
1	K	195	PHE	2.4
1	M	195	PHE	2.4
1	D	159	THR	2.4
1	I	72	LYS	2.4
1	M	96	ILE	2.4
1	K	161	PRO	2.4
1	K	136	GLN	2.3
1	G	66	ARG	2.3
1	E	209	ASP	2.3
1	B	30	VAL	2.3
1	A	72	LYS	2.3
1	K	193	LEU	2.3
1	I	97	VAL	2.3
1	A	74	ALA	2.3
1	A	96	ILE	2.3
1	A	222	ILE	2.3
1	E	207	LEU	2.3
1	D	222	ILE	2.3
1	M	215	ALA	2.3
1	B	13	ASN	2.3
1	K	96	ILE	2.3
1	J	223	LYS	2.3
1	I	183	GLY	2.3
1	K	107	ARG	2.3
1	L	160	ARG	2.2
1	C	70	ASP	2.2
1	M	174	ASP	2.2
1	A	223	LYS	2.2
1	D	37	TYR	2.2
1	I	213	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	218	ILE	2.2
1	J	191	GLU	2.2
1	F	203	ARG	2.2
1	H	30	VAL	2.2
1	F	74	ALA	2.2
1	J	58	GLU	2.2
1	D	200	ILE	2.2
1	L	221	SER	2.2
1	M	221	SER	2.2
1	G	223	LYS	2.2
1	M	72	LYS	2.2
1	G	22	MET	2.2
1	D	218	ILE	2.2
1	F	16	ILE	2.2
1	A	71	PHE	2.2
1	I	73	VAL	2.1
1	F	17	LEU	2.1
1	L	217	GLY	2.1
1	J	96	ILE	2.1
1	B	193	LEU	2.1
1	F	167	LEU	2.1
1	C	72	LYS	2.1
1	E	72	LYS	2.1
1	B	34	VAL	2.1
1	K	143	ALA	2.1
1	I	174	ASP	2.1
1	K	192	THR	2.1
1	H	223	LYS	2.1
1	A	224	ASP	2.1
1	B	72	LYS	2.1
1	F	160	ARG	2.1
1	M	66	ARG	2.1
1	F	63	PHE	2.1
1	F	199	ILE	2.1
1	L	208	ALA	2.0
1	G	73	VAL	2.0
1	C	68	ILE	2.0
1	G	96	ILE	2.0
1	L	62	ARG	2.0
1	K	151	VAL	2.0
1	L	147	VAL	2.0
1	L	183	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	224	ASP	2.0
1	B	36	GLU	2.0
1	L	29	ARG	2.0
1	M	191	GLU	2.0
1	K	164	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	2OM	C	229	24/24	0.92	0.29	1.45	62,65,66,68	0
2	2OM	A	229	24/24	0.97	0.28	1.39	49,62,68,70	0
2	2OM	I	229	24/24	0.74	0.39	1.00	69,73,76,77	0
2	2OM	E	229	24/24	0.91	0.19	0.09	67,69,72,73	0
2	2OM	B	229	24/24	0.87	0.18	0.06	68,69,72,73	0
2	2OM	J	229	24/24	0.89	0.18	0.05	67,70,71,72	0
2	2OM	H	229	24/24	0.88	0.16	-0.23	68,71,74,76	0
2	2OM	F	229	24/24	0.78	0.20	-0.27	67,71,75,76	0
2	2OM	M	229	24/24	0.87	0.18	-0.41	66,69,71,72	0
2	2OM	G	229	24/24	0.90	0.16	-0.58	67,71,73,74	0
2	2OM	K	229	24/24	0.91	0.13	-0.60	68,71,73,74	0
2	2OM	D	229	24/24	0.88	0.16	-0.68	69,71,73,74	0
2	2OM	L	229	24/24	0.85	0.16	-0.84	70,72,74,75	0



## 6.5 Other polymers

There are no such residues in this entry.